LBM 20th Oct 2016

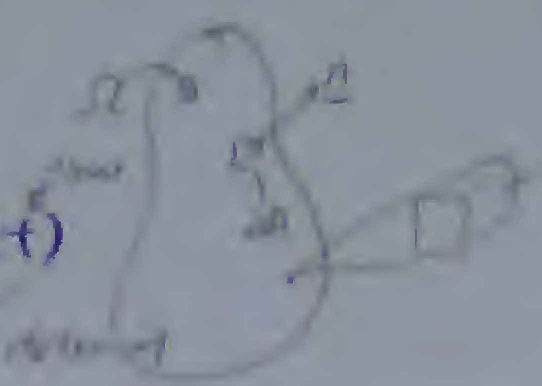
1 Continuum Mechanics.

Goal: Derive Navier Stokes equations in $\mathbb{R}^3$

assume density is a point-defined ... such as an average of gas molecules contained in dV

(1.1) Control Volume

w.l.o.g. $\Omega \neq \Omega(t)$



dV $dm = \rho(x)\, dV$

Knudsen number: $\dfrac{\lambda}{L}$ (mean f.p. / characteristic length)

Consider Rate of Change of (...)

i. mass.

$$\frac{d}{dt}\int_\Omega \rho\, dV = -\int_{\partial\Omega} \rho\, \underline{u}\cdot\underline{n}\, dA \qquad (1)$$

ii. momentum (Newton), $i = 1,2,3$ direction, $\underline{u} = (u_1, u_2, u_3)^T$

$$\frac{d}{dt}\int_V \rho u_i\, dV$$

$$= -\int_{\partial\Omega} (\rho u_i)\, \underline{u}\cdot\underline{n}\, dA + \int_{\partial\Omega} t_i\, dA \;;\; t_i = \sigma_{ij} n_j = \begin{bmatrix} \sigma_{1j} n_j \\ \sigma_{2j} n_j \\ \sigma_{3j} n_j \end{bmatrix} = \sum_{j=1}^{3} \sigma_{ij} n_j$$

(summation convention)

$\underline{\underline{\sigma}} = (\sigma_{ij})_{ij=1,2,3}$ stress tensor (symm.)

$\sigma_{ij} = -P\delta_{ij} + \tau_{ij}$

diagonal (principal), off-diagonal (shear stress)

$$\Rightarrow \boxed{\frac{d}{dt}\int_V \rho u_i\, dV = -\int_{\partial\Omega} \rho u_i\, \underline{u}\cdot\underline{n}\, dA - \int_{\partial\Omega} p\,\underline{n}\, dA + \int_{\partial\Omega} \underline{\underline{\tau}}\, \underline{n}\, dA} \qquad (2)$$

iii. Energy:

$$\frac{d}{dt}\int E\, dV = -\int_{\partial\Omega} E\, \underline{u}\cdot\underline{n}\, dA - \int_{\partial\Omega} p\, \underline{u}\cdot\underline{n}\, dA + \int_{\partial\Omega} (\underline{\underline{\tau}}\, \underline{u})\cdot\underline{n}\, dA - \int_{\partial\Omega} \underline{q}\cdot\underline{n}\, dA \qquad (3)$$

Use Divergence Theorem:

(i) $\displaystyle\int_{\Omega} \frac{d}{dt}\rho\, dV + \int_\Omega \nabla\cdot(\rho\underline{u})\, dV = 0$ $\qquad \frac{d}{dt}\rho + \nabla\cdot(\rho\underline{u}) = 0$

(ii) $\displaystyle\int_\Omega \left(\frac{\partial \rho \underline{u}}{\partial t} + \nabla\cdot(\rho\,\underline{u}\otimes\underline{u}) + \nabla p - \nabla\cdot\underline{\underline{\tau}}\right) dV = 0$; $\underline{u}\otimes\underline{u} = (u_i u_j)$ $i,j = 1,2,3$

(iii) $\displaystyle\int_\Omega \left(\frac{\partial E}{\partial t} + \nabla\cdot(E\underline{u}) + \nabla\cdot(p\underline{u}) - \nabla\cdot(\underline{\underline{\tau}}\,\underline{u}) + \nabla\cdot\underline{q}\right) dV = 0$

can't solve the three pdes, as there are 15 unknowns but 5 eqs.

To close the system:

(1.2) Equation of state:

$P = \rho R T$, R - specific gas constant.

$R = c_p - c_v$ heat capacity at constant p & v

$= c_v \left(\frac{c_p}{c_v} - 1 \right)$; $\gamma = \frac{c_p}{c_v}$

$\Rightarrow RT = (\gamma - 1) c_v T$ e_{int} (specific int. energy) "calorically perfect gas" } followed by ideal gas assumption

Now:

energy per unit volume

$E = \rho e_{int} + \frac{1}{2} \rho \|u\|^2$

internal energy, kin. energy

$\Rightarrow \rho e_{int} = E - \frac{1}{2} \rho \|u\|^2$

by ideal gas law:

$P = \rho \underbrace{(\gamma-1) c_v T}_{RT} = \rho (\gamma - 1) e_{int} = (\gamma - 1) \left(E - \frac{1}{2} \rho \|u\|^2 \right)$, hence we reduced an unknown 'P'

$p = \rho R T$; $R = \frac{J}{kg \cdot K} = \frac{\hat{R}}{M}$ universal gas constant, molar mass, $[M] = \frac{kg}{mol}$ (mass of 1 mol)

$p = \rho \frac{\hat{R}}{M} T$; $M = m \cdot N_A$ avogadro's constant, mass of one molecule

$= \rho \frac{\hat{R}}{m N_A} T$

ρ / m: number density, $\hat{R}/N_A$: k_B Boltzmann constant

Finally: $p = n k_B T$ in this representation, it doesn't matter which species of gas is dynamic, what matters is just the number of molecules in the gas

(1.3) ~~Consecutive laws~~

Constitutive Laws.

(i) Newtonian Fluids.

$\tau_{ij} = C_{ijkl} \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)$

4th order tensor

We may:

- homogeneity
- isotropy.

$\Rightarrow C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$

$\Rightarrow \tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k}$ — As a result, τ depends only on u & x!

often: $\lambda = -\frac{2}{3} \mu$ "Stokes Hypothesis"

chosen such that τ_{ij} is traceless, $\tau_{ii} = 0$, should note that after substituting the principal stresses are not affected.

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(ii) Fourier's Law

$$\underline{q} = -k \nabla T$$ from $\rho T = (\gamma - 1)(E - \frac{1}{2}\rho \|u\|^2)$

coefficient of heat conduction

hence, we reduced another unknown $\underline{q}$

~~Inc~~ Incompressible N-S

$$\nabla \cdot \underline{u} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \ ; \ \nu = \frac{\mu}{\rho_0}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{u}) = 0 \ ; \quad \nabla = \frac{\partial^2}{\partial x_j \partial x_j}$$

LBM 27th Oct 2016 (tutorial)

Intro to Probability Theory

(1) Sample space and Probability.

(1.1) $\Omega := \{$ "All possible Outcomes of an Experiment" $\}$

Example

(E1) $\Omega := \{1, 2, 3, 4, 5, 6\}$ to roll a die

(E2) $\Omega := \{$"heads", "tails"$\}$ to flip a coin

(E3) $\Omega := \{1, 2, 3, \ldots\} \equiv \mathbb{N}$ How many time until we get red? (in roulette)

For now: finite or countably infinite sample space

(1.2) Events $A \subset \Omega$

Example: (E1) "Even number" $A = \{2, 4, 6\} \subset \Omega$

Elementary event: Singleton set containing only one element $\omega \in \Omega$ $A = \{\omega\}$

(1.3) Probability : $\mathbb{P} : \mathcal{P}(\Omega) \to [0,1]$

power set, set of all sets

probability of everything = any events

s.th : $\mathbb{P}(\Omega) = 1$

finite Ω : $\mathbb{P}(A_1) + \mathbb{P}(A_2) = \mathbb{P}(A_1 \cup A_2)$, $A_1 \cap A_2 \cancel{\neq} = \emptyset$

infinite Ω : $\sum_{n=1}^{\infty} P(A_i) = P(\bigcup_{n=1}^{\infty} A_n)$

(σ - additivity)

We call $(\Omega, \mathbb{P})$ a probability space.

Example:

E1 "Even number" $A_1 = \{2, 4, 6\}$

"Odd number" $A_2 = \{1, 3, 5\}$

If we assume ~~$P(\{w_i\}) = \frac{1}{6}$~~ ~~$i = 1, \dots, 6$~~ $P(\{w_i\}) = \frac{1}{6}$, $i = 1, \dots, 6$

Then $P(A_1) = \frac{1}{2} = P(A_2)$

$P(A_1) + P(A_2) = 1 = P(A_1 \cup A_2)$

Probability Function

$\mathbb{P}(\{w_i\}) = p(w_i)$

$\rightarrow \quad 1 = \sum_{w \in \Omega} p(w)$

"probability of elementary events"

Example: AKA (Laplace model $p(w) = \frac{1}{\# \Omega}$, $p(A) = \frac{\# A}{\# \Omega}$)

E1 $p(w) = \frac{1}{6} \quad \forall w = \Omega$

E2 $p(w) = \frac{1}{2} \quad \forall w \in \Omega$

E3 $p(1) = \frac{18}{37}$ ← # red balls / ← all balls

$p(2) = \frac{19}{37} \cdot \frac{18}{37}$

$p(3) = \left(\frac{19}{37}\right)^2 \cdot \frac{18}{37}$

$p(n) = \left(\frac{19}{37}\right)^{n-1} \cdot \frac{18}{37}$

(1.5) Probability: $P : \mathcal{P}(\Omega) \to [0,1]$

1st: $P(\Omega) = 1$

2nd: $P(A_1) + P(A_2) = P(A_1 \cup A_2)$, $A_1 \cap A_2 = \emptyset$

infinite Ω: $\sum_{n=1}^{\infty} P(A_n) = P\left(\bigcup_{n=1}^{\infty} A_n\right)$

(σ-additivity)

We call (Ω, P) a probability space

Example:

(E1) "Even number" $A_1 = \{2, 4, 6\}$

"Odd number" $A_2 = \{1, 3, 5\}$

If we stand ~~$P(\{\omega\}) = \frac{1}{6}$~~ ~~$i = 1, \dots, 6$~~ $P(\{\omega_i\}) = \frac{1}{6}$, $i = 1, \dots, 6$

thus $P(A_1) = \frac{1}{2} = P(A_2)$

$P(A_1) + P(A_2) = 1 = P(A_1 \cup A_2)$

Probability Function

$P(\{\omega\}) = p(\omega)$

$\Rightarrow 1 = \sum_{\omega \in \Omega} p(\omega)$

"probability of elementary events"

Example: $p(\omega) = \frac{1}{\#\Omega}$, $P(A) = \frac{\#A}{\#\Omega}$

(E1) $p(\omega) = \frac{1}{6} \quad \forall \omega \in \Omega$

(E2) $p(\omega) = \frac{1}{2} \quad \forall \omega \in \Omega$

(E3) $p(1) = \frac{18}{37}$

$p(2) = \frac{19}{37} \cdot \frac{18}{37}$

$p(3) = \left(\frac{19}{37}\right)^2 \cdot \frac{18}{37}$

$p(n) = \left(\frac{19}{37}\right)^{n-1} \cdot \frac{18}{37}$

⑤

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① Check:

$$\sum_{n=1}^{\infty} p(n) = \frac{18}{37} \sum_{r=0}^{\infty} \Big(\underbrace{\frac{19}{37}}_{q<1}\Big)^r$$

$$= \frac{18}{37} \cdot \frac{1}{1-q}$$ geometric series

$$= 1$$

(1.4) Multivariate Probability

$$\Omega^n = \Omega \times \Omega \times \Omega \dots \times \Omega := \{(a_1, \dots, a_n) : a_i \in \Omega\}$$

Example "Two dice"

$$\Omega^2 = \Omega \times \Omega := \{(a_1, a_2) : a_i \in \Omega\}$$

$$w_i \in \Omega^2 = (a_1, a_2) \quad a_i \in \{1, 2, 3, 4, 5, 6\}$$

$$p(w_i) = \frac{1}{36}$$

② Random variables

$$X : \Omega \to \mathbb{R}$$

$$p(X = a) = P(a) = \sum_{\substack{w \in \Omega \\ X(w) = a}} p(w)$$

function that takes elementary events (w) as input, that gives new events

Example: E1 "two dice"

$$w = (i, j) \quad i, j = 1, \dots, 6$$

$$X(w) = i + j$$

$$\{w \in \Omega : X(w) = 5\} = \{X = 5\} = \{(1,4), (4,1), (3,2), (2,3)\}$$

$$P(X = 5) = \frac{4}{36} = \frac{1}{9}$$

(E2) $\{$"heads", "tails"$\}$

$X(\text{"heads"}) = +1$

$X(\text{"tails"}) = -1$

(E1) $X(w) = \begin{cases} -2000 & w = \{1,2,3,4\} \\ +5000 & w = \{5,6\} \end{cases}$ ← would you play?

(e.g. die)

(3) moments

(3.1) Expectation values

~~expected~~ outcome of event

$$\mu(X) = \sum_{w \in \Omega} X(w)\, p(w)$$

expectation value function

probability of the event

Consider above (E1),

$$\mu(X) = \sum_{w \in \Omega} -2000 \cdot \frac{2}{3} + 5000 \cdot \frac{1}{3} \approx +333$$

(3.2) $\mu(F(x)) = \sum_{w \in \Omega} F(X(w))\, p(w)$

e.g. $\mu(X^k) = \sum_{w \in \Omega} X^k p(w)$

Example: variance   outcome   expected outcome

$$\sigma^2(X) = \mu((X - \mu(X))^2)$$

of event!!!

$$= \mu(X^2 - 2X\mu(X) + \mu(X)^2)$$ apply the function to each of the terms

$$= \mu(X^2) - 2\mu(X)\mu(X) + \mu(X)^2$$ expectation value of a constant is the constant itself

$$= \mu(X^2) - \mu(X)^2$$

(3.3) standardized distribution

$$X \mapsto X^* = \frac{X - \mu(X)}{\sigma(X)} \Rightarrow \mu(X) = 0$$

4 Information Entropy

(4.1) "Self - Information" or "Surprise"

negative

$$I(\omega) = -\log_b(p(\omega)) \geq 0$$

Example:

$p(\omega) = 1 \Rightarrow I(\omega) = 0$

$p(\omega) \to 0 \Rightarrow I(\omega) \to \infty$

Let $b = 2$, for event (E2)

$\Omega := \{$"heads", "tails"$\}$

$p(\omega) = \frac{1}{2}$

$I(\omega) = 1$

(4.2) Information Entropy $\to$ $H = \mu(I) = -\sum_{\omega \in \Omega} p(\omega) \log(p(\omega))$

(E2) $\Omega := \{$"heads", "tails"$\}$

(i) "Fair coin" $p(\omega) = \frac{1}{2}$

$H = 1$ $\left(\sum_{\omega \in \Omega} \frac{1}{2} (-1) \right)$

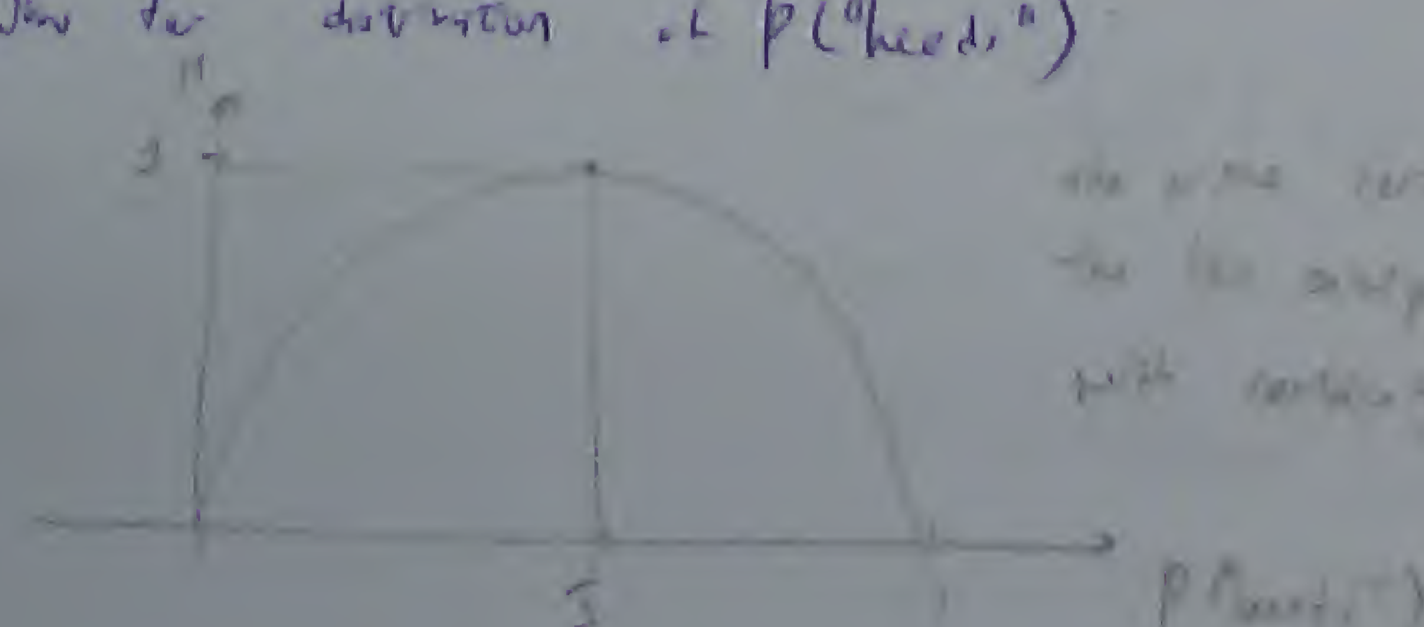
(ii) "unfair coin"

$p($"heads"$) = 1$

$p($"tails"$) = 0$

$H = 0$

Now for distribution of $p($"heads"$)$



the more certain of the outcome, the less entropy is has with certainty, $H \to 0$

5 Continuous Sample Space

(5.1) probability density function.

$$f : \mathbb{R} \to [0, \infty)$$

$$\int_{\mathbb{R}} f \, dx = 1$$

$$P(a \leq X \leq b) = \int_a^b f \, dx$$

Example: Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(\frac{-(x-\mu)^2}{\sigma^2}\right) =: N(\mu, \sigma)$$

Multivariate case:

$$f : \mathbb{R}^n \to [0, \infty)$$

$$\underline{x} = (x_1, \ldots, x_n)$$

$$\int_{\mathbb{R}^n} f \, dx_1 \ldots dx_n = 1$$

(5.2) $$\mu(x) = \int_{\mathbb{R}} x\, f(x)\, dx$$

multivariate case:

$$\mu(x_k) = \int_{\mathbb{R}} x_k\, f(\underline{x})\, \underbrace{dx_1 \cdots dx_n}_{d\underline{x}}$$

(5.3) Entropy

$$H(f) = -\int_{\mathbb{R}^n} f \ln(f)\, d\underline{x}$$ — H theorem

6 Central limit theorem

Consider (E2) $\Omega = \{\text{"heads"}, \text{"tails"}\}$

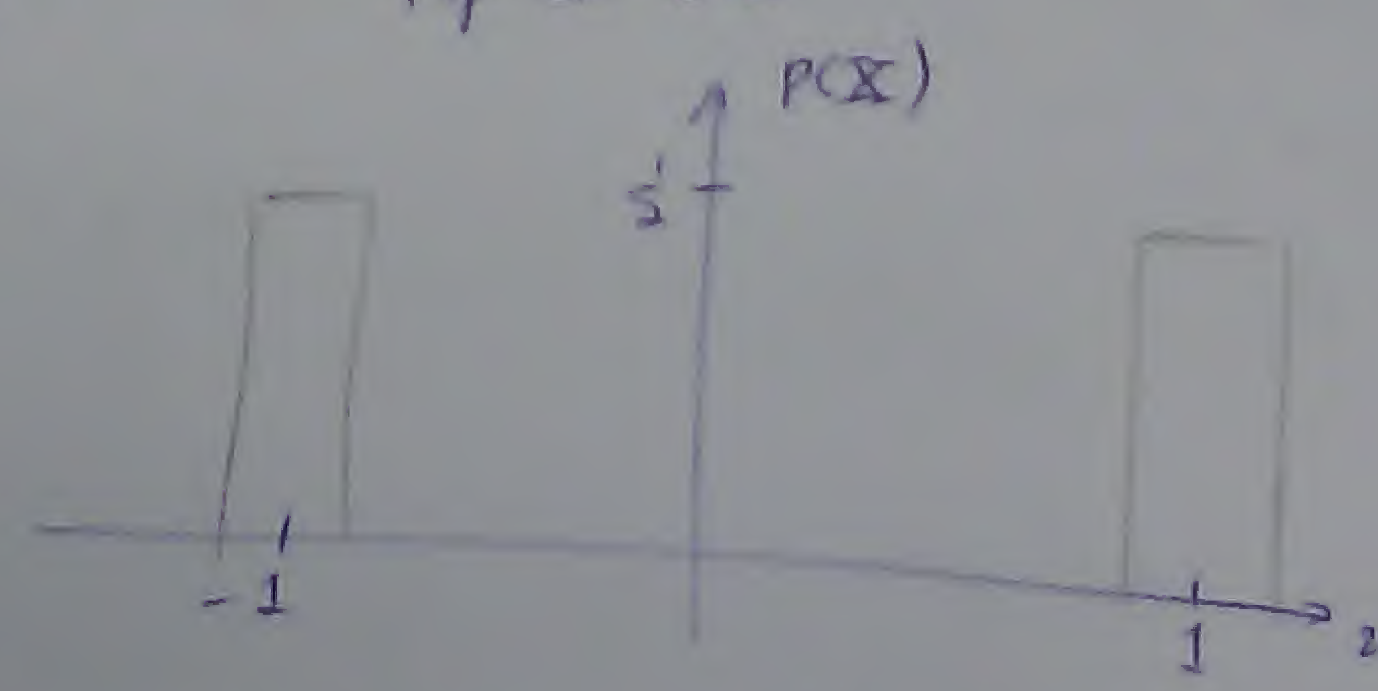
$p(\omega) = \frac{1}{2} \quad \omega \in \Omega$

$\underline{X}(\text{"heads"}) = -1$

$\underline{X}(\text{"tails"}) = +1$

$\mu(\underline{X}) = 0$ rule (3.1)

Flip coin once



Flip twice:

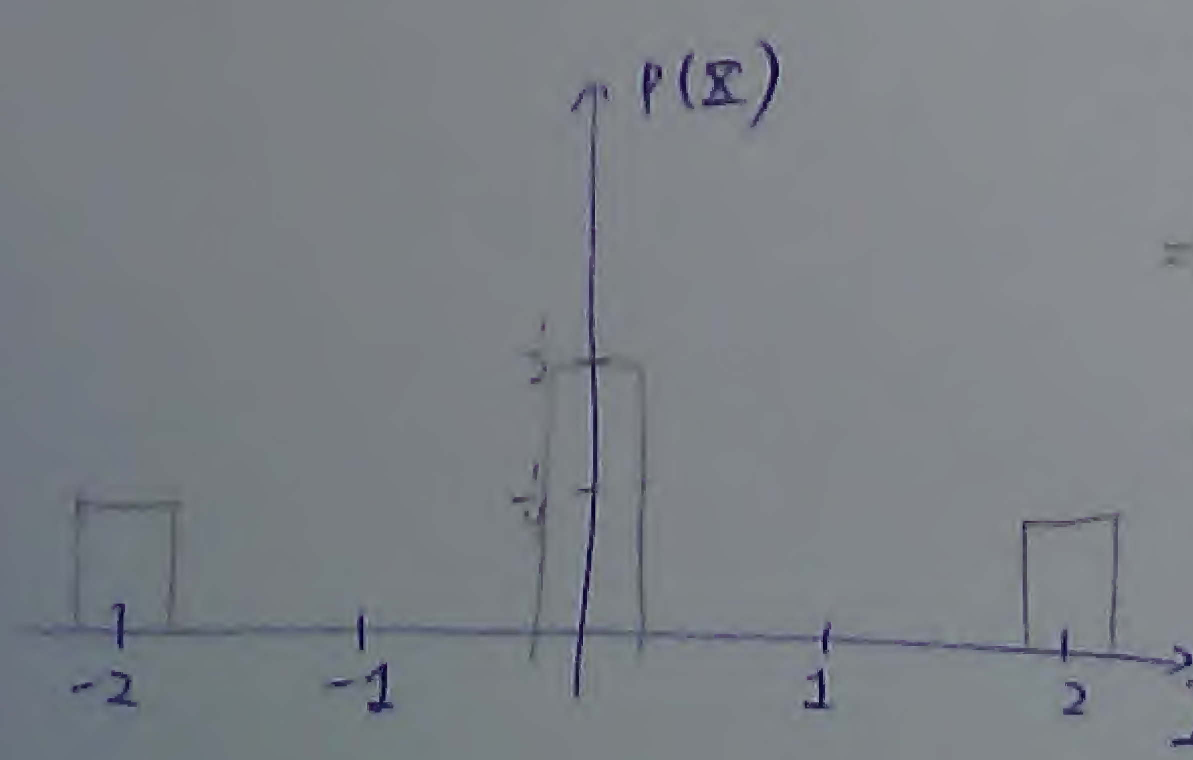
$\Omega^2 = \Omega \times \Omega$

$:= \{(a_1, a_2) : a_i \in \Omega\}$

$\underline{X}(a_1) = \underline{X}_1$

$\underline{X}(a_2) = \underline{X}_2$

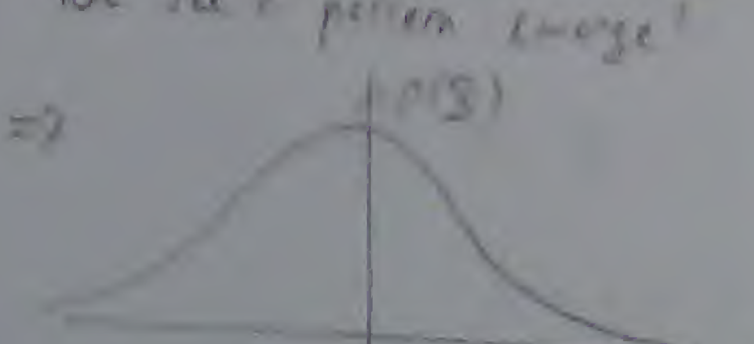
$\underline{X} = \underline{X}_1 + \underline{X}_2$



$\underline{X} = \underline{X}_1 + \underline{X}_2$

as number of flips increases, we see a pattern emerge!

$\Rightarrow$



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same Laplacian model each time experiment is done

Let $X_1, \ldots, X_n$ be independent, identically distributed (iid) random variables

$$a_n = S_n = X_1 + \ldots + X_n$$

$$\lim_{n\to\infty} \left(\frac{S_n - \mu(S_n)}{\sigma(S_n)} \right) = N(0,1) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2} \right)$$

doesn't have to be Laplacian model, as long as model stays the same and independent to each other

LBM 28th Oct 2016

(Ch. 4. The Maxwell-Boltzmann Distribution

"gas in a box"

$\rho = \rho_0 = \text{const.}$

$T = T_0 = \text{const.}$

etc.

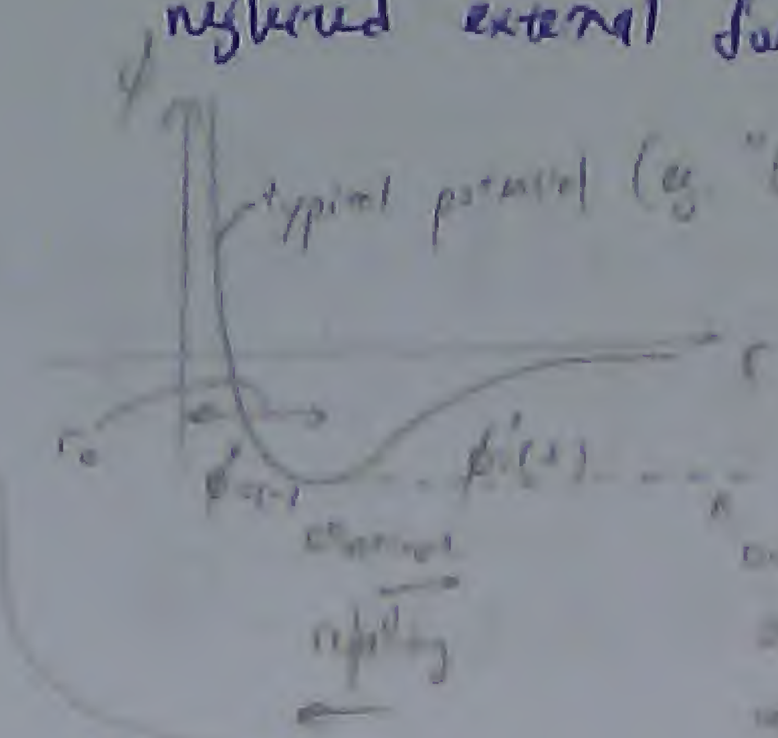
neglected external forces.

We assume:

* binary interactions.
* Spherically symmetric potentials. } not restrictions but for convenience

$$F = -\phi'(r)$$

force, potential



our assumption: no interaction over large distances
only interacting under collision
(billiard ball model)

(4.1) intermolecular interactions

Consider two particles

$m_A, \underline{c}$ @ $t=0$ $\underline{x}_A$ - location

$m_B, \underline{z}$ $\qquad \underline{x}_B$

velocity

$\underline{c} = \dot{\underline{x}}_A$

$$\underline{x}_m = \frac{\underline{x}_A m_A + \underline{x}_B m_B}{m_A + m_B}$$

"centre of mass"

$$\Rightarrow \underline{w} = \dot{\underline{x}} = \frac{\dot{\underline{x}}_A m_A + \dot{\underline{x}}_B m_B}{m_A + m_B}$$

$$= \frac{\underline{c} m_A + \underline{z} m_B}{m_A + m_B}$$

Note: const velocity ($\underline{w} = \text{const.}$)

Consider reference frame moving with velocity $\underline{w}$

$$\hat{\underline{c}} := \underline{c} - \underline{w} = -\mu_B \underline{g} \;(1); \quad \underline{g} = \underline{z} - \underline{c}$$

$$\hat{\underline{z}} := \underline{z} - \underline{w} = \mu_A \underline{g} \;(2)$$

$$\mu_i = \frac{m_i}{m_A + m_B} \quad i = A, B$$

$$m_A \hat{\underline{c}}(t) \underset{(1),(2)}{=} -m_B \hat{\underline{z}}(t)$$

$$\Rightarrow m_A \|\underline{c}\| = m_B \|\underline{z}\| \quad \forall (t)$$

Relation between

$\hat{\underline{c}}, \hat{\underline{z}}$ and $\hat{\underline{c}}', \hat{\underline{z}}'$

before, after

Let $\hat{c} = \|\hat{\underline{c}}\|$

$\hat{z} = \|\hat{\underline{z}}\|$

we have

$$m_A \hat{c} = m_B \hat{z}$$

$$m_A \hat{c}' = m_B \hat{z}'$$

$$\Rightarrow m_A(\hat{c} + \hat{c}') = m_B(\hat{z} + \hat{z}') \quad (3)$$

$$m_A(\hat{c} - \hat{c}') = m_B(\hat{z} - \hat{z}') \quad (4)$$

Kinetic Energy:

$$\frac{1}{2} m_A \hat{c}^2 + \frac{1}{2} m_B \hat{z}^2 = \frac{1}{2} m_A (\hat{c}')^2 + \frac{1}{2} m_B (\hat{z}')^2$$

Note:

$$m_A = m_B \Rightarrow \begin{matrix} \hat{c} = \hat{c}' \\ \hat{z} = \hat{z}' \end{matrix}$$

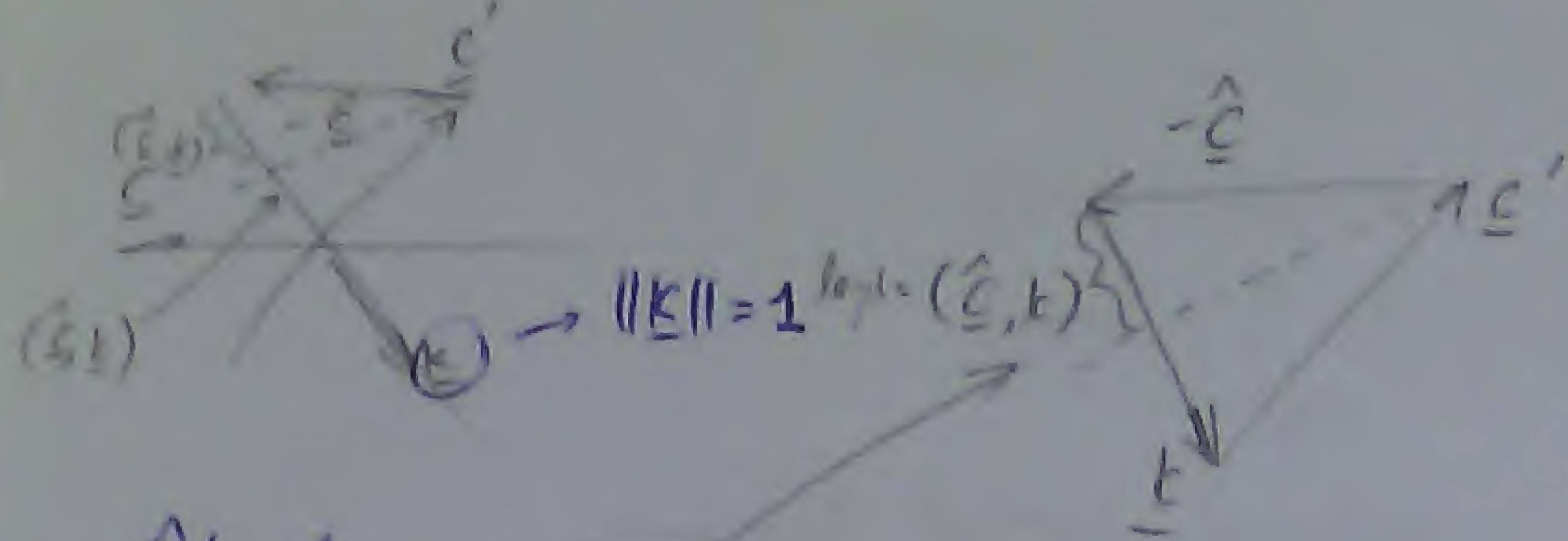
Let $m_A \neq m_B$, see notes.

again, we have $\hat{c} = \hat{c}'$, $\hat{z} = \hat{z}'$

Conservation of angular momentum:

$b = b'$ (see figure, take moment about (B))

also: planar motion.



$$\hat{\underline{c}}' - \hat{\underline{c}} = -(\hat{\underline{c}}, \underline{k})\underline{k} \cdot 2$$

$$= \cancel{A} - 2(\underbrace{\underline{c} - \underline{w}}_{\mu_B \underline{g}}, \underline{k})\,\underline{k} = +2\mu_B(\underbrace{\underline{z} - \underline{c}}_{\underline{g}}, \underline{k})\,\underline{k}$$

note! no hat!

$$\underline{c}' = \underline{c} + 2\mu_B(\underline{z} - \underline{c}, \underline{k})\underline{k} \quad (*)$$

$$\underline{z}' = \underline{z} - 2\mu_A(\underline{z} - \underline{c}, \underline{k})\underline{k} \quad (**)$$

$$\begin{pmatrix} \underline{c}' \\ \underline{z}' \end{pmatrix} = \underline{F}(\underline{c}, \underline{z}) = \begin{pmatrix} \underline{F}_1(\underline{c}, \underline{z}) \\ \underline{F}_2(\underline{c}, \underline{z}) \end{pmatrix} \begin{array}{l} (*) \\ (**) \end{array}$$

Jacobian:

3×3 matrix

$$F' = \left(\begin{array}{c|c} \dfrac{\partial \underline{F}_1}{\partial \underline{c}} & \dfrac{\partial \underline{F}_1}{\partial \underline{z}} \\ \hline \dfrac{\partial \underline{F}_2}{\partial \underline{c}} & \dfrac{\partial \underline{F}_2}{\partial \underline{z}} \end{array}\right)$$

$\det F' = 1$

LBM 3rd Oct 2016 tutorial

1 Integral Transformation

Motivation:

Let $D := \{(x,y) : x^2+y^2 \le R^2,\ R>0\}$ (*)

Consider:

$$\iint_D f(x,y)\,dx\,dy = \int_{-R}^{R}\int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2+y^2}} f(x,y)\,dx\,dy$$

Let $\Phi : S \to D$ be a coordinate transformation.

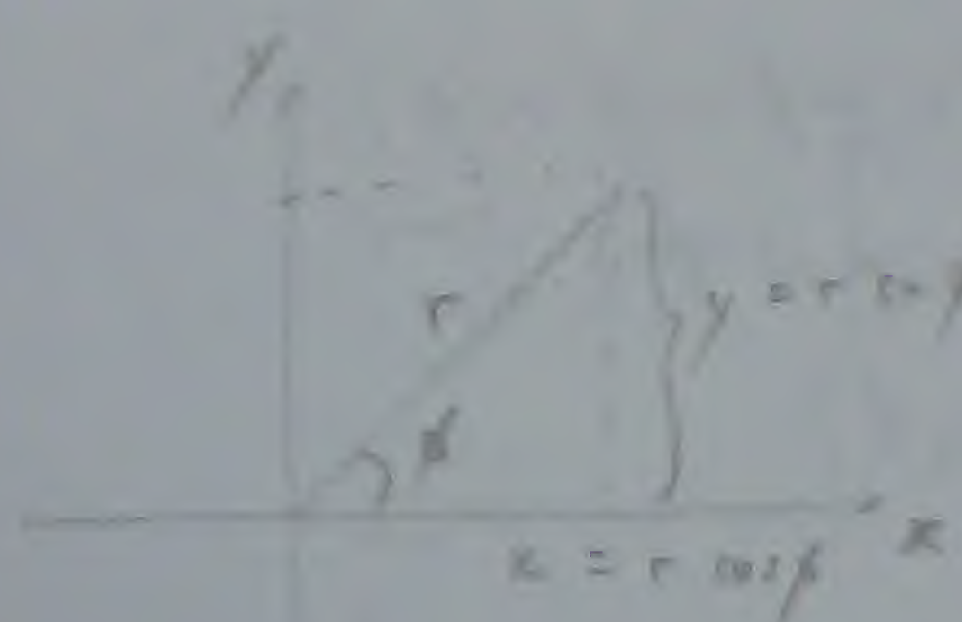
$(u,v) \longmapsto \Phi(u,v) = (x,y)$

$(u,v,w) \longmapsto \Phi(u,v,w) = (x,y,z)$

Example (a) polar coordinates

$u = r$

$v = \phi$



$$\Phi = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$$

$x = r\cos\phi$

$y = r\sin\phi$

$$\begin{bmatrix} dx \\ dy \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \phi} \end{bmatrix} \begin{bmatrix} dr \\ d\phi \end{bmatrix}$$

$$\begin{bmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{bmatrix}$$

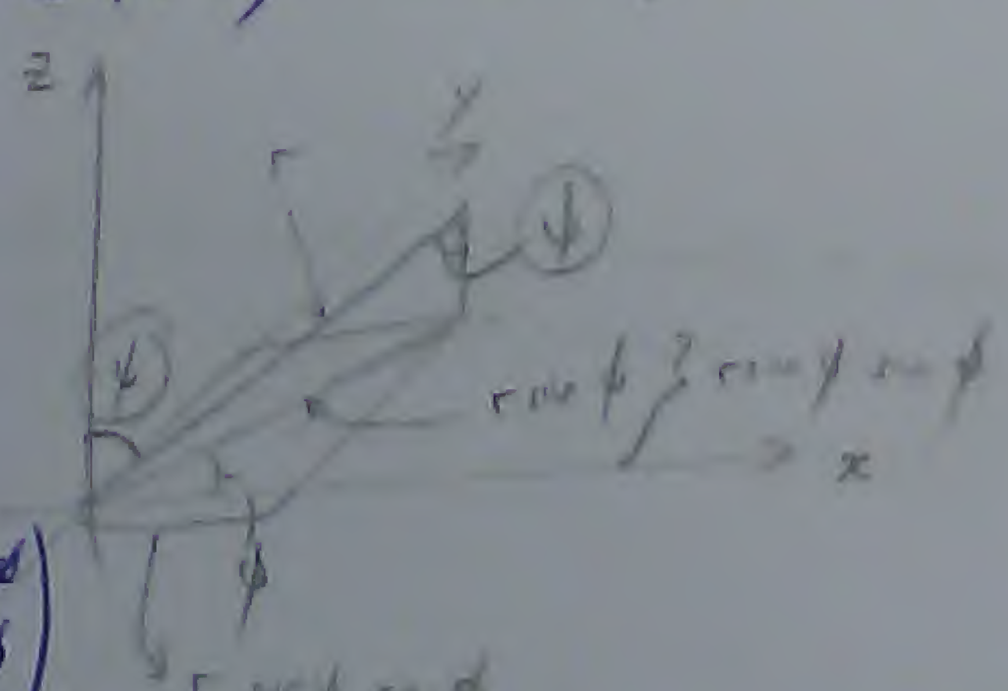
consider D as in (*)

Then $S = [0,R] \times [0,2\pi)$ for bijection, as $0, 2\pi$ for the free direction maps to the same value.

(b) $u = r$

$v = \phi$

$w = \psi$

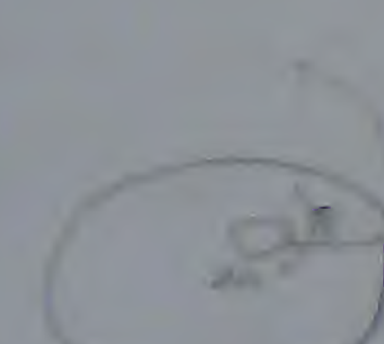


$x = r\sin\psi\cos\phi$

$y = r\sin\psi\sin\phi$

$z = r\cos\psi$

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} & ? & \end{bmatrix} \begin{bmatrix} dr \\ d\phi \\ d\psi \end{bmatrix}$$



$$\Phi(r,\phi,\psi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$$

$D := \{(x,y,z) : x^2+y^2+z^2 \le R^2\}$ $\quad S := [0,R] \times [0,\pi] \times [0,2\pi]$

$$\int_D dx\,dy\,dz = \int_S |\det \Phi'|\,dr\,d\phi\,d\psi$$

u

z

Example.

ⓐ $\Phi(r,\phi) = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$

$\Phi'(r,\phi) = \begin{pmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{pmatrix}$

$\det \Phi' = r(\cos^2\phi + \sin^2\phi)$

$= r$

$$\Rightarrow \int_D dx\,dy = \int_0^{2\pi}\int_0^R r\,dr\,d\phi$$

$$= 2\pi \int_0^R r\,dr$$

$$= \pi\left[\frac{1}{2}r^2\right]_0^R$$

$$= \pi R^2$$

②

ⓑ $\Phi(r,\psi,\phi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$ $\quad \Phi'(r,\psi,\phi) = \begin{pmatrix} \sin\psi\cos\phi & r\cos\psi\cos\phi & -r\sin\psi\sin\phi \\ \sin\psi\sin\phi & r\cos\psi\sin\phi & r\sin\psi\cos\phi \\ \cos\psi & -r\sin\psi & 0 \end{pmatrix}$

$$\det\Phi'(r,\psi,\phi) = r^2\cos\psi(\cos\psi\sin\psi\cos^2\phi + \sin\psi\cos\psi\sin^2\phi)$$
$$+ r^2\sin\psi(\sin^2\psi\cos^2\phi + \sin^2\psi\sin^2\phi)$$
$$= r^2(\cos^2\psi\sin\psi + \sin\psi\sin^2\psi)$$
$$= r^2\sin\psi$$

$\rightarrow dx\,dy\,dz = r^2\sin\psi\,dr\,d\psi\,d\phi$

② Recursion formulae

for: $\displaystyle\int_0^\infty x^n e^{-ax^2}dx =: I_n$

① $I_0 = \displaystyle\int_0^\infty e^{-ax^2}dx$ — formally, to proceed, we need to determine if the integral is finite. in e^{-x} form, at infinity, the polynomial x^n will be [illegible], similarly, at $x=0$, polynomial [illegible] out e^{-x} function so it is finite

$$I_0^2 = \int_0^\infty e^{-ax^2}dx \int_0^\infty e^{-ay^2}dy$$

$x = r\cos\phi$
$y = r\sin\phi$

$$\Rightarrow = \int_0^\infty\int_0^\infty e^{-a(x^2+y^2)}dx\,dy$$

$0 \to x \to \infty$, $0 \to y \to \infty$; $\cos\phi / \sin\phi \in [-1,1]$, but in our integration domain, $[0,\infty]$: $\cos\phi \to [0,1]$ $\Rightarrow \phi \to [0,\frac{\pi}{2}]$

$$= \int_0^{\frac{\pi}{2}}\int_0^\infty e^{-ar^2}r\,dr\,d\phi$$

$$= \frac{\pi}{2}\int_0^\infty e^{-ar^2}r\,dr \quad (**)$$

$z = ar^2 \quad dz = 2ar\,dr$

$$= \frac{\pi}{2}\frac{1}{2a}\int_0^\infty e^{-z}dz = \frac{\pi}{4a}(-e^{-z})\Big|_0^\infty = \frac{\pi}{4a} \Rightarrow I_0 = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

(ii) $I_1 = \int_0^\infty x e^{-ax^2}\,dx \overset{(**)}{=} \frac{1}{2a}$

$\int_0^\infty x e^{-ax^2}\,dx$ previously $\Rightarrow \frac{1}{2a}$

(iii) Consider:

$$\frac{d}{da} I_n = \frac{d}{da}\int_0^\infty x^n e^{-ax^2}\,dx$$

$$= \int_0^\infty x^n \frac{d}{da} e^{-ax^2}\,dx$$

$$= -\int_0^\infty x^{n+2} e^{-ax^2}\,dx = -I_{n+2}$$

Iden tity: (recursion)

$$\boxed{I_n = \cancel{-\tfrac{d}{da}} - \frac{d}{da} I_{n-2} \qquad n = 2, 3, 4, \ldots}$$

Example:

$I_2 = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$

$I_3 = \frac{1}{2a^2}$

$I_4 = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}$

Remark: $\tilde{I}_n = \int_{-\infty}^\infty x^n e^{-ax^2}\,dx$

$\tilde{I}_n = 0$ (n odd)

$\tilde{I}_n = 2 I_n$ (n even)

$x \cdot e^{-ax^2}$, the resulting product ... integrating the whole ... the ... evenly

(3) gaussian / maxwellian

Let $\hat{f}(c)$ be p.d.f.

normalise

$f(c) = n \hat{f}(c)$ number density, $[n] = m^{-3}$

Note:

$n = \int_{\mathbb{R}^3} f(c)\,dc$ velocity space

or $1 = \int_{\mathbb{R}^3} \hat{f}(c)\,dc$

We define:

$\underline{u} \overset{(A)}{=} \frac{1}{n}\int_{\mathbb{R}^3} c f(c)\,dc$ "bulk velocity"

expectation value of velocity, gives a factor of n, so $\frac{1}{n}$ is there to normalise it

$$\frac{3}{2} k_B T = \frac{1}{n}\int_{\mathbb{R}^3} \frac{m}{2}\underbrace{|u-c|^2}_{\text{"thermal velocities"}} f(c)\,dc$$

Tomorrow: In equilibrium

$$f(c) = A e^{-\beta^2 |c-\alpha|^2}$$

Consider

$$n \doteq \int_{\mathbb{R}^3} f(\underline{c})\, d\underline{c} \qquad f(\underline{c}) = A\, e^{-\beta^2 |\underline{c}-\underline{\alpha}|^2}$$

$$\underline{\xi} = \underline{c} - \underline{\alpha} \qquad d\underline{\xi} = d\underline{c} \qquad d\underline{\xi} = [d\xi_1, d\xi_2, d\xi_3]$$

$$\Rightarrow n = \int_{\mathbb{R}^3} f(\underline{\xi})\, d\underline{\xi} \qquad e^{-\beta \xi_1}\, e^{-\beta \xi_2^2}\, e^{-\beta \xi_3^2}$$

$$= A \int_{\mathbb{R}^3} e^{-\beta^2 \{\xi_1^2 + \xi_2^2 + \xi_3^2\}}\, d\xi_1\, d\xi_2\, d\xi_3$$

$$= A \underbrace{\left(\int_{\mathbb{R}} e^{-\beta^2 \xi^2}\, d\xi \right)^3}_{I_0 \ (a = \beta^2)}$$

$$\to \boxed{I_0 = \frac{\pi^{3/2}}{|\beta|^3}}$$

$$\Rightarrow n = A \cdot \frac{\pi^{3/2}}{|\beta|^3}$$

$$\Rightarrow A = \frac{n |\beta|^3}{\pi^{3/2}}$$

Can work out $\alpha = u$ using (4)

Also: $$\frac{3}{2} k_B T = \frac{m}{2} A \int_{\mathbb{R}^3} \xi^2 e^{-\beta^2 \xi^2}\, d\underline{\xi}$$

$$= \frac{m}{2} A \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \xi^4 e^{-\beta^2 \xi^2} \sin\psi\, d\psi\, d\phi\, d\xi$$

$$\Rightarrow 3 k_B T = m A \cdot 2\pi \underbrace{\int_0^{\pi} \sin\psi\, d\psi}_{= -\cos\psi |_0^{\pi} = 2} \underbrace{\int_0^{\infty} \xi^4 e^{-\beta^2 \xi^2}\, d\xi}_{= I_4 \ (a = \beta^2)}$$

$$I_4 = \frac{3}{8} \sqrt{\frac{\pi}{|\beta|^5}}$$

$$\beta^2 = \frac{m}{2 k_B T}, \quad A = \frac{n}{(2\pi R T)^{3/2}}$$

$$k_B = \frac{\hat{R}}{N_A} = \frac{R M}{N_A} = R \cdot m$$

Maxwell – Boltzmann

$$f(\underline{c}) = \frac{n}{(2\pi R T)^{3/2}}\, e^{\left(-\frac{|\underline{c}-\underline{u}|^2}{2RT} \right)}$$

Compare to standard gaussian:

$$N^3(\mu, \sigma) = \frac{1}{(2\pi)^{3/2} \sigma^3} \exp\left\{ \frac{-|\underline{x} - \underline{\mu}|^2}{2\sigma^2} \right\}$$

$$\sigma^2 = RT$$

$$\mu_i = u_i, \quad i = 1, 2, 3.$$

LBM ~~4th Oct 2013~~ 4th Nov 2016

(4.2) Equilibrium velocity distribution

1. basic definitions

Postulate ~~$\hat{f}(\underline{c})$~~ $\hat{f}(\underline{c})$ such that

molecular velocities

$$\int_{\mathbb{R}^3} \hat{f}(\underline{c}) \underbrace{dc_1\, dc_2\, dc_3}_{d\underline{c}} = 1$$

Hence $\hat{f}(\underline{c})\,d\underline{c}$ is probability that a molecule has velocity between c_i and $c_i + dc_i$ $(i=1,2,3)$

We use:

$$f(\underline{c}) = n\hat{f}(\underline{c}) \quad \rightarrow \rho = m \cdot n$$

mass of molecule

We define:

$$\underline{u} = \frac{1}{n}\int_{\mathbb{R}^3} \underline{c}\, f(\underline{c})\, d\underline{c} = 0$$

under equilibrium assumption

$$\frac{3}{2}k_B T = \int_{\mathbb{R}^3} \frac{m}{2}|u - c|^2 f(\underline{c})\, d\underline{c}$$

$$= \int_{\mathbb{R}^3} \frac{m}{2}\xi^2 f(\xi)\, d\xi \; ; \; \xi = \underline{c} - \underline{u} \,,\; \xi^2 = |\xi|^2$$

2. How to find f?

Equilibrium assumption: $\frac{\partial}{\partial t}\{f(\underline{c})\,d\underline{c}\} = 0$ $(f \neq f(x))$

* only mechanism changing $f(\underline{c})$: collisions.

* $\underbrace{\text{"depleting" collisions}}_{\text{I}}$ and $\underbrace{\text{"replenishing" collisions}}_{\text{II}}$

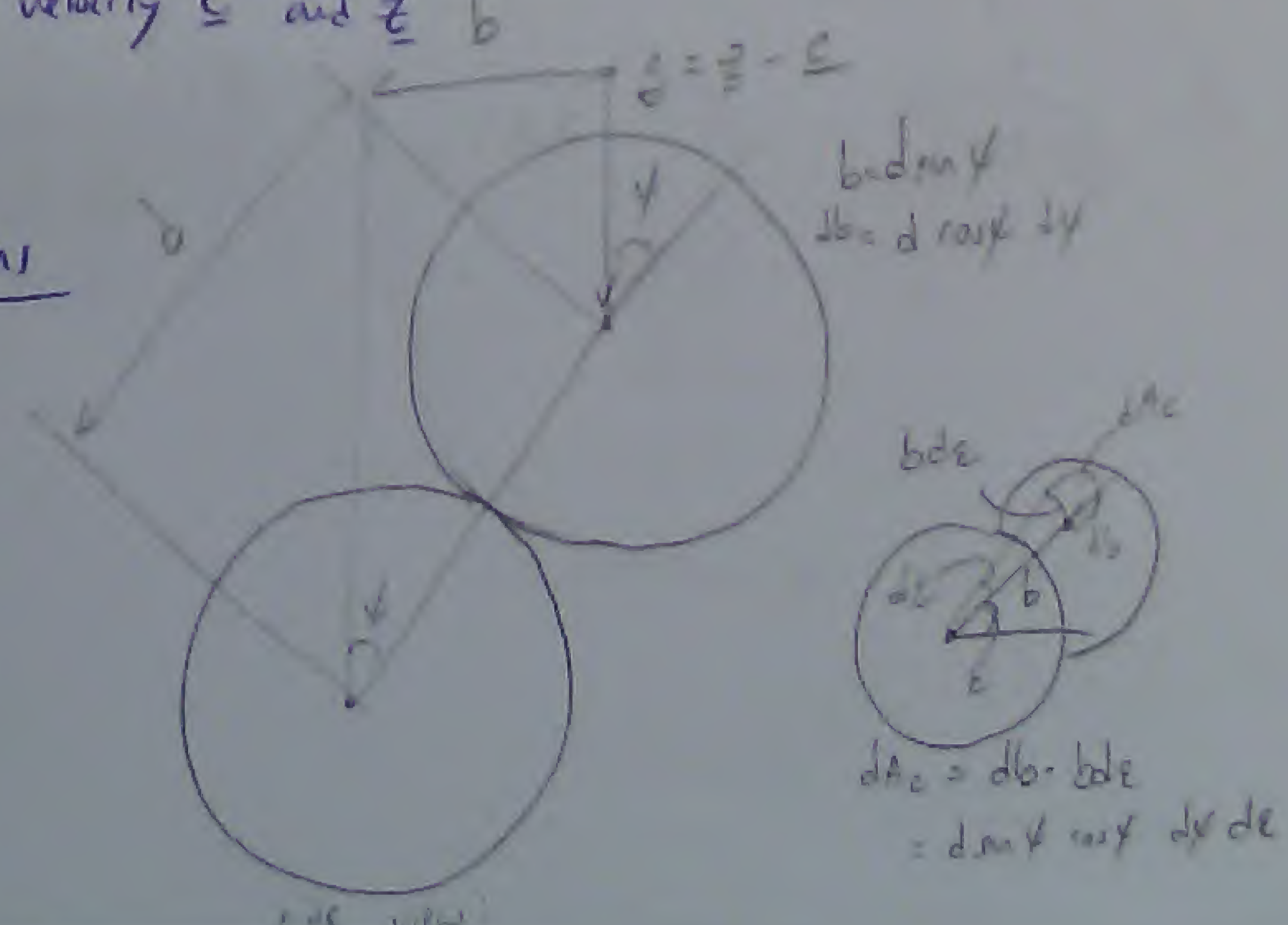
I Consider collision between molecules having velocity $\underline{c}$ and $\underline{z}$

A priori assumption

$$\frac{\partial}{\partial t}\{f(\underline{c})\,d\underline{c}\} \propto f(\underline{c})\,d\underline{c} \times \frac{\#\text{ collisions}}{dt}$$

more molecule that travel in velocity $\underline{c}$,
more chance of collision with other velocity $\underline{z}$,
more rate of change

We reference frame with velocity $\underline{c}$:



$dV_c := g\,dt \cdot dA_c$ unit area = volume covered by particle moving in velocity $\underline{g} = \underline{z} - \underline{c}$
distance travelled

All particle (with velocity $\underline{z}$) inside dV_c

i.e $f(\underline{z})\,d\underline{z}\,dV_c$

will hit our particle with velocity $\underline{c}$ during

same, hence $\underline{c}/\underline{z} = -(\underline{c}/\underline{z})$ doesn't matter the direction (+/−). symmetry, here $\int_0^{\pi} \to \int_0^{\pi/2}$ for $d\psi$

$$\Rightarrow \frac{\partial f(\underline{c})\,d\underline{c}}{\partial t} \quad (2) = \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, g(\underline{c},\underline{z})\, f(\underline{c}) f(\underline{z}) \sin\psi \cos\psi \; d\psi\, d\varepsilon\, d\underline{c}\, d\underline{z}$$

$$\Rightarrow \frac{\partial\{f(\underline{c})\,d\underline{c}\}}{\partial t} \quad (1) = \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, g(\underline{c}',\underline{z}')\, \underset{\substack{\Downarrow \\ \underline{F}_1(\underline{c},\underline{z})}}{f(\underline{c}')} f(\underline{z}') \sin\psi\cos\psi\; d\psi\, d\varepsilon\, d\underline{z}'\, d\underline{c}'$$

collision change of velocity (reverse)

$$= \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, g(\underline{c},\underline{z})\, f(F_1(\underline{c},\underline{z})) f(F_2(\underline{c},\underline{z})) \sin\psi\cos\psi\; d\psi\, d\varepsilon\, d\underline{z}\, d\underline{c}\; \overbrace{|\det F'|}^{=1}$$

$$\to \frac{\partial f(\underline{c})}{\partial t} = \iiint g(\underline{c},\underline{z}) \Big(f(\overbrace{F_1(\underline{c},\underline{z})}^{c'})\, f(\overbrace{F_2(\underline{c},\underline{z})}^{z'}) - f(\underline{c}) f(\underline{z}) \Big) \overbrace{dA_c}^{d^2\sin\psi\cos\psi\, d\psi\, d\varepsilon}\, d\underline{z}$$

detailed balanced $= 0$

note, we don't integrate over $d\underline{c}$, because we only account for particles in $\underline{c}$ velocity.

$$\to f(\underline{c}') f(\underline{z}') = f(\underline{c}) f(\underline{z})$$

$$\log f(\underline{c}') + \log f(\underline{z}') = \log f(\underline{c}) + \log f(\underline{z})$$

before & after collisions, quantity must be conserved. that means $\log f(\underline{c})$ is a linear combination of conserved quantities, that is mass, momentum, energy (m, mv, $\frac{1}{2}v^2$ velocity)

So $\log f(\underline{c})$ must be of the form

$$\log f(\underline{c}) = a + b_1 c_1 + b_2 c_2 + b_3 c_3 + \frac{\tilde{a}}{2}|\underline{c}|^2$$

in other words, $\log f(\underline{c}) = \mathrm{span}\{1, \underline{v}, \frac{|\underline{v}|^2}{2}\}$

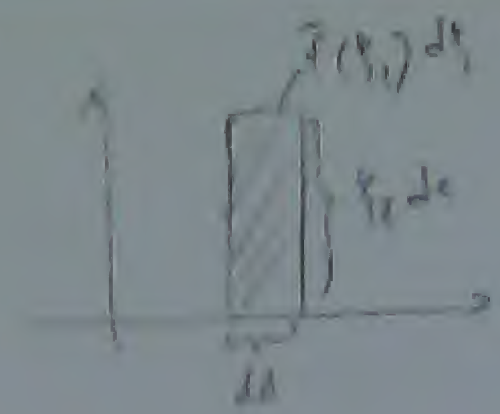
$$= -\beta^2\left((c_1-\alpha_1)^2 + (c_2-\alpha_2)^2 + (c_3-\alpha_3)^2\right) + \alpha_0$$

$$\Rightarrow f(\underline{c}) = e^{-\beta^2|\underline{c}-\underline{\alpha}|^2}\, e^{\alpha_0} = A$$

We showed yesterday:

$$A = \frac{n}{(2\pi RT)^{3/2}} \qquad \beta^2 = \frac{1}{2RT} \qquad \underline{\alpha} = \underline{u}$$

Note! The whole derivation of $f(\underline{c})$ in this lecture is dependent on the assumption that the gas is in equilibrium! If the assumption doesn't hold, then $f(\underline{c})$ is unknown!



Winter Semester 2016/17

Lattice-Boltzmann Methods

Prof. Georg May

Tutorial 3

Problem 1

Derive an expression for the thermodynamic pressure as the mean flux of the molecular "thermal" momentum $m\boldsymbol{\xi}$. (Here $\boldsymbol{\xi} = \mathbf{c} - \mathbf{u}$ is the thermal vecocity, given by the difference between the molecular velocity $\mathbf{c}$ and the bulk fluid velocity $\mathbf{u}$.)

Problem 2

Compute the mean velocity *magnitude* for a gas in thermodynamic equilibrium from the Maxwell-Boltzmann distribution.

Problem 3

Compute the mean free path of a molecule of a gas in thermodynamic equilibrium, using the Maxwell-Boltzmann distribution.

Problem 2

$$\hat{f}(c) = \frac{1}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} e^{-\frac{|\xi|^2}{2RT}} \, d\xi$$

$$= \frac{1}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} |\xi| \, e^{-\frac{|\xi|^2}{2RT}} \, d\xi$$

$$J_n(a) = \int_0^\infty x^n e^{-ax^2} dx \quad (a>0)$$

$$\sqrt{\frac{8RT}{\pi}}$$

$$c = \sqrt{\gamma RT}$$

Problem 3

$$\frac{1}{n}\int_{\mathbb{R}^3} \frac{\partial f(\xi)}{\partial t}\, d\xi \Big|_I =: \nu$$ no. of collisions per unit time

direction: $d^2 \sin\psi\cos\psi \; d\varepsilon\, d\psi$

$$\nu = \frac{1}{n}\int_{A_c}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g(\xi,\zeta)\, f(\xi)\, f(\zeta)\, dA_c\, d\zeta\, d\xi$$

Since f is Maxwellian:

$$= \frac{1}{n}\frac{n^2 d^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_0^{2\pi}\int_0^{\pi/2} g(\xi,\zeta)\, e^{-\frac{|\xi|^2+|\zeta|^2}{2RT}} \sin\psi\cos\psi\, d\psi\, d\varepsilon\, d\xi\, d\zeta$$

$$\int_0^{\pi/2} \sin\psi\cos\psi\, d\psi = \sin^2\psi\Big|_0^{\pi/2} - \int_0^{\pi/2}\sin\psi\cos\psi\, d\psi$$ now by IBP

$$= \frac{1}{2}\sin^2\psi\Big|_0^{\pi/2} = \frac{1}{2}$$

$$\int_0^{2\pi} d\varepsilon = 2\pi$$

$$\Rightarrow \nu = \frac{\pi d^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g(\xi,\zeta)\, e^{-\frac{|\xi|^2+|\zeta|^2}{2RT}}\, d\xi\, d\zeta \; ; \; g = |\mathbf{g}|,$$ magnitude of $\zeta - \xi = \mathbf{g}$

Consider:

$\mathbf{g} = \zeta - \xi \Rightarrow \zeta = \mathbf{g} + \xi$ (a)

$\boxed{w = \frac{1}{2}(\zeta + \xi)} = \frac{1}{2}(\mathbf{g} + 2\xi)$

$\Rightarrow \xi = w - \frac{1}{2}\mathbf{g}$ (b)

substitute (b) into (a)

$\Rightarrow \zeta = w + \frac{1}{2}\mathbf{g}$ (c)

$F : \mathbb{R}^6 \to \mathbb{R}^6$

$$F(w,\mathbf{g}) = \begin{pmatrix} F_1(w,\mathbf{g}) \\ F_2(w,\mathbf{g}) \end{pmatrix} \begin{matrix} (b) \\ (c) \end{matrix} \qquad \begin{matrix} \xi = F_1(w,\mathbf{g}) \\ \zeta = F_2(w,\mathbf{g}) \end{matrix}$$

3x3 mat

$$\Rightarrow F' = \begin{pmatrix} \frac{\partial \xi}{\partial w} & \frac{\partial \xi}{\partial \mathbf{g}} \\ \frac{\partial \zeta}{\partial w} & \frac{\partial \zeta}{\partial \mathbf{g}} \end{pmatrix} = \begin{pmatrix} I & -\frac{1}{2}I \\ I & \frac{1}{2}I \end{pmatrix}$$

$$|\det F'| = |\det(\tfrac{1}{2}I + \tfrac{1}{2}I)| = 1$$

Now: $|\xi|^2 + |\zeta|^2 = (w - \frac{1}{2}\mathbf{g}, w - \frac{1}{2}\mathbf{g}) + (w + \frac{1}{2}\mathbf{g}, w + \frac{1}{2}\mathbf{g})$

$= 2|w|^2 + \frac{1}{2}|\mathbf{g}|^2$

$$\nu = \frac{\pi d^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g\, e^{-\frac{(2|w|^2+\frac{1}{2}|\mathbf{g}|^2)}{2RT}}\, d\mathbf{g}\, dw \Rightarrow \underbrace{\int_{\mathbb{R}^3} g\, e^{-\frac{|\mathbf{g}|^2}{4RT}}\, d\mathbf{g}}_{(d)} \underbrace{\int_{\mathbb{R}^3} e^{-\frac{|w|^2}{RT}}\, dw}_{(e)}$$

$$(d) = 4\pi\underbrace{\int_0^\infty g^3 e^{-\frac{g^2}{4RT}}\, dg}_{I_3(\frac{1}{4RT})} = 8(RT)^2 \qquad (e) = 4\pi\underbrace{\int_0^\infty w^2 e^{-\frac{w^2}{RT}}\, dw}_{I_2(\frac{1}{RT})} = (\pi RT)^{3/2}$$

$\Rightarrow \nu = 4nd^2\sqrt{\pi RT}$; time between collision, $\tau = \frac{1}{\nu}$ | $\lambda = \bar{c}\tau = \bar{c}/\nu = \sqrt{\frac{8RT}{\pi}}\cdot\frac{1}{\nu} = \frac{1}{\sqrt{2}\,\pi n d^2}$

LBM 11th Nov 2016

Chapter 5: The Boltzmann Equation.

In the non-equilibrium case.

$$f = f(\underline{c}, \underline{x}, t)$$

$$n(x,t) = \int_{\mathbb{R}^3} f(\underline{c}, \underline{x}, t)\, d\underline{c}$$

$$u(x,t) = \frac{1}{n(x,t)} \int_{\mathbb{R}^3} \underline{c}\, f(\underline{c}, \underline{x}, t)\, d\underline{c}$$

Boltzmann Equation

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$$

$$J(f,f) = \int_{A_c} \int_{\mathbb{R}^3} g(\underline{c}, \underline{z}) \left(f(\underline{c}') f(\underline{z}') - f(\underline{c}) f(\underline{z}) \right) dA_c\, d\underline{z}$$

Can show:

$$\int_{\mathbb{R}^3} \phi(\underline{c})\, J(f,f)\, d\underline{c} = 0 \quad ; \left(J(f,f) \sim \frac{\partial f}{\partial t}\Big|_{coll.} \right)$$

$$\text{for } \phi(\underline{c}) = \begin{cases} m \\ m\underline{c} \\ \frac{1}{2} m |\underline{c}|^2 \end{cases}$$

collisional invariants.

literally, there is not net change in the conserved quantities due to collision

Take moments of Boltzmann Equations:

$$\int_{\mathbb{R}^3} \phi(c) \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} - J(f,f) \right\} d\underline{c} = 0$$

(1) $\phi(\underline{c}) = m$

$$\Rightarrow \int_{\mathbb{R}^3} \phi(\underline{c}) \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\Rightarrow \int_{\mathbb{R}^3} m \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} m \underbrace{\int_{\mathbb{R}^3} f(\underline{c})\, dc}_{n} + \frac{\partial}{\partial x_\alpha} m \underbrace{\int_{\mathbb{R}^3} c_\alpha f(\underline{c})\, dc}_{n u_\alpha} = 0$$

look above!

$\rho = m \cdot n$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha} (\rho u_\alpha) = 0$$

(ii) $\phi(\underline{c}) = m c_\alpha$

$$\Rightarrow \int_{\mathbb{R}^3} m c_\alpha \left(\frac{\partial f}{\partial t} + c_\beta \frac{\partial f}{\partial x_\beta} \right) d\underline{c} = 0$$

Indices, as it indicates a tensor.

$$\Rightarrow \frac{\partial}{\partial t} m \underbrace{\int_{\mathbb{R}^3} c_\alpha f(c) d\underline{c}}_{n u_\alpha} + \frac{\partial}{\partial x_\beta} m \int_{\mathbb{R}^3} c_\alpha c_\beta f(c) d\underline{c} = 0$$

Recall: $\underline{c} = \underline{u} + \underline{\xi}$

$$\Rightarrow \frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\alpha} m \int_{\mathbb{R}^3} (u_\alpha + \xi_\alpha)(u_\beta + \xi_\beta) \tilde{f}(\xi) d\xi = 0$$

(deviation)

0, average of deviation to velocity = 0

(Check!)

$$\Rightarrow \frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\alpha} m \Big\{ \underbrace{\int_{\mathbb{R}^3} u_\alpha u_\beta \tilde{f}(\xi) d\xi}_{n} + \int_{\mathbb{R}^3} \xi_\alpha u_\beta \tilde{f}(\xi) d\xi + \int_{\mathbb{R}^3} u_\alpha \xi_\beta \tilde{f}(\xi) d\xi + \underbrace{\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \tilde{f}(\xi) d\xi}_{P_{\alpha\beta} = m \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \tilde{f}(\xi) d\xi} \Big\} = 0$$

$$\int_{\mathbb{R}^3} \xi_\alpha \tilde{f}(\xi) d\xi = 0$$

expectation value of velocity fluctuations

(iii) $\phi(\underline{c}) = \frac{1}{2} m c^2$

$$\int_{\mathbb{R}^3} \frac{1}{2} m c^2 \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\underbrace{\frac{\partial}{\partial t} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 f(c) d\underline{c}}_{(a)} + \underbrace{\frac{\partial}{\partial x_\alpha} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 c_\alpha f(c) d\underline{c}}_{(b)} = 0$$

Note: $c^2 = (\underline{u} + \underline{\xi}, \underline{u} + \underline{\xi})$

$= \underline{u}^2 + 2(\underline{\xi}, \underline{u}) + \xi^2$

(a) $= \frac{\partial}{\partial t} \frac{m}{2} \int_{\mathbb{R}^3} (u^2 + \xi^2) f(\xi) d\xi$

$$= \frac{\partial}{\partial t} \underbrace{\left(\frac{m}{2} n u^2 + \overbrace{\int \frac{m}{2} \xi^2 f(\xi) d\xi}^{= \frac{3}{2} n k_B T} \right)}_{E}$$

(b) $\frac{\partial}{\partial x_\beta} \left\{ \frac{m}{2} \int_{\mathbb{R}^3} (\xi_\beta + u_\beta)(u^2 + 2\xi_\alpha u_\alpha + \xi^2) f(\xi) d\xi \right\}$

$$= \frac{\partial}{\partial x_\beta} \Big\{ \underbrace{\frac{m}{2} \int_{\mathbb{R}^3} 2 \xi_\alpha \xi_\beta u_\alpha f(\xi) d\xi}_{P_{\alpha\beta} U_\alpha} + \underbrace{\frac{m}{2} \int_{\mathbb{R}^3} \xi_\beta \xi^2 f(\xi) d\xi}_{q_\beta}$$

$$\underbrace{+ \frac{m}{2} u^2 u_\beta \underbrace{\int_{\mathbb{R}^3} f(\xi) d\xi}_{n} + \underbrace{\frac{m}{2} \int_{\mathbb{R}^3} u_\beta \xi^2 f(\xi) d\xi}_{u_\beta \cdot \frac{3}{2} n k_B T}}_{E u_\beta} \Big\}$$

(a) + (b) $\Rightarrow \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_\beta}(E u_\beta) + \frac{\partial}{\partial x_\beta}(P_{\alpha\beta} U_\alpha) + \frac{\partial q_\beta}{\partial x_\beta} = 0$

Assume: Local thermodynamic equilibrium

$$f(\underline{c}, \underline{x}, t) = \frac{n(x,t)}{(2\pi R T(x,t))^{3/2}} e^{\frac{-|c - u(x,t)|^2}{2RT(x,t)}}$$

Consider:

$$P_{\alpha\beta} = \int_{\mathbb{R}^3} m \xi_\alpha \xi_\beta f(\xi) d\xi = \overbrace{\frac{nm}{(2\pi RT)^{3/2}}}^{A} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta e^{\frac{-|\xi|^2}{2RT}} d\xi$$

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(i) $\alpha \neq \beta$

$$P_{\alpha\beta} = A \int_{\mathbb{R}^3} \xi_\alpha e^{-\frac{\xi_\alpha^2}{2RT}} d\xi \int_{\mathbb{R}^3} \xi_\beta e^{-\frac{\xi_\beta^2}{2RT}} d\xi \int_{\mathbb{R}^3} e^{-\frac{\xi_\gamma^2}{2RT}} d\xi$$

$\to 0$, since odd!

$$(\alpha, \beta, \gamma) = \sigma(1,2,3) \quad \text{permutation}$$

$$P_{\alpha\beta} = 0 \quad (\alpha \neq \beta)$$

(ii) $\alpha = \beta$

$$P_{\alpha\alpha} = A \int_{\mathbb{R}^3} m\xi_\alpha^2 e^{-\frac{\xi_1^2+\xi_2^2+\xi_3^2}{2RT}} d\xi$$

$$= \underbrace{\frac{A}{3} \int_{\mathbb{R}^3} m \underbrace{(\xi_1^2+\xi_2^2+\xi_3^2)}_{\xi^2} e^{-\frac{\xi^2}{2RT}} d\xi}_{p}$$

$$\Rightarrow q_\beta = \int \frac{m}{2} \xi^2 \xi_\beta f(\xi)\, d\xi$$

$$= \frac{\rho}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} \xi^2 \xi_\beta e^{-\frac{\xi^2}{2RT}} d\xi$$

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} \xi \sin\psi \cos\phi \\ \xi \sin\psi \sin\phi \\ \xi \cos\psi \end{pmatrix}$$

spherical coordinates:

$$q_\beta = A \iiint \xi^2 \underbrace{\xi \cdot h(\psi,\phi)}_{\xi_\beta} e^{-\frac{\xi^2}{2RT}} \xi^2 \sin\psi\, d\psi\, d\phi\, d\xi$$

$h(\psi,\phi)$

$$\Rightarrow q_\beta = A \int_0^\infty \xi^5 e^{-\frac{\xi^2}{2RT}} \underbrace{\int_0^\pi \int_0^{2\pi} h(\psi,\phi) \sin\psi\, d\psi\, d\phi}_{(*)}$$

eg. $\beta = 2$, $h(\psi,\phi)_2 = \sin\psi \sin\phi$

$$\Rightarrow (*) = \int_0^\pi \sin^2\psi\, d\psi \underbrace{\int_0^{2\pi} \sin\phi\, d\phi}_{0}$$

$\beta = 3$

$$\Rightarrow (*) = \int_0^\pi \sin\psi \cos\psi\, d\psi = \frac{1}{2} \sin^2\psi \Big|_0^\pi = 0$$

hence $q = 0$ if f is maxwellian.

$$\Rightarrow \frac{\partial\rho}{\partial t} + \frac{\partial(\rho u_\alpha)}{\partial x_\alpha} = 0$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} + \frac{\partial p}{\partial x_\alpha} = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial(E u_\beta)}{\partial x_\beta} + \frac{\partial p u_\beta}{\partial x_\beta} = 0$$

f is locally Maxwellian.

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Today:

1. Collisional invariants
2. Boltzmann H-theorem

① Recall: Collision Integral:

$$J(f,f) = \int_{\mathbb{R}^3}\int_{A_c} g(\underline{c},\underline{z})\big(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\big)\, d\underline{z}\, dA_c \;;\; \underline{c}'(\underline{c},\underline{z};\psi,\varepsilon)$$

collision angle

$$\underline{z}'(\underline{c},\underline{z};\psi,\varepsilon)$$

$$\underline{F} = \begin{pmatrix} \underline{F}_1(\underline{c},\underline{z};\psi,\varepsilon) \\ \underline{F}_2(\underline{c},\underline{z};\psi,\varepsilon)\end{pmatrix} \qquad \underline{F}_1' = \underline{c}' \qquad \underline{F}_2' = \underline{z}'$$

$$\underline{F}_1 = \underline{c} + 2\mu_B(\underline{g},\underline{k}(\psi,\varepsilon))\,\underline{k}(\psi,\varepsilon)$$

$$\underline{F}_2 = \underline{z} - 2\mu_A(\underline{g},\underline{k}(\psi,\varepsilon))\,\underline{k}(\psi,\varepsilon)$$

$$\mu_i = \frac{m_i}{m_A+m_B} \qquad i = A, B$$

$$m_A = m_B \Rightarrow \mu_i = \frac{1}{2}$$

Boltzmann Eqn:

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$$

Consider: moments:

$$I_\phi := \int_{\mathbb{R}^3} J(f,f)\phi(\underline{c})\, d\underline{c}$$

$$\rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{c},\underline{z})\big(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\big)\phi(\underline{c})\, d\underline{c}\, d\underline{z}\, dA_c \qquad (1)$$

Now, trivially exchange variable names $\underline{c} \leftrightarrow \underline{z}$

$$\rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{z},\underline{c})\big(f(\underline{c}'(\cdot)),f(\underline{z}'(\cdot)) - f(\underline{z})f(\underline{c})\big)\phi(\underline{z})\, d\underline{c}\, d\underline{z}\, dA_c$$

$$\underline{c}' = \underline{c}'(\underline{z},\underline{c},\psi,\varepsilon)$$

$$\underline{z}' = \underline{z}'(\underline{z},\underline{c},\psi,\varepsilon)$$

Now consider physical symmetries

$$\underline{g}(\underline{c},\underline{z}) = -\underline{g}(\underline{z},\underline{c}) \qquad \text{also: } \underline{c}'(\underline{c},\underline{z}) = \underline{z}'(\underline{z},\underline{c})$$

$$\Rightarrow g(\underline{c},\underline{z}) = g(\underline{z},\underline{c}) \qquad \underline{z}'(\underline{c},\underline{z}) = \underline{c}'(\underline{z},\underline{c})$$

$|\underline{g}|$ $\qquad$ from ⊛

(2)

$$\Rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(c,z)\left(f(c'(c,z))f(z'(c,z)) - f(c)f(z)\right)\phi(z)\, dc\, dz\, dA_c$$

We can now write:

$$I_\phi = \frac{1}{2}\left((1) + (2)\right)$$

Similarly can rewrite twice more

$$\Rightarrow I_\phi = \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(c,z)\left(f(c')f(z') - f(c)f(z)\right)\left(\phi(c)+\phi(z) - \phi(c') - \phi(z')\right) dc\, dz\, dA_c$$

$I_\phi = 0$ for $\phi(c)$ s.th. $\phi(c) + \phi(z) = \phi(c') + \phi(z')$

true for: $\phi(c) = \begin{cases} m \\ mc \\ \frac{m}{2}c^2 \end{cases}$

② H - Theorem:

$$H = -\int_{\mathbb{R}^3} f \ln f \, dc \qquad \text{Assume } f \equiv f(c,t)$$

We show

(i) $\frac{dH}{dt} \geq 0$ and $\frac{dH}{dt} = 0$ iff f is Maxwellian.

(ii) H is entropy

(ii) Consider Entropy of closed system.

$$T\,dS = dE + p\,dV$$

ideal gas := $p = nk_BT$

$$= \frac{N}{V}k_BT$$

$$e = \frac{3}{2}nk_BT \Rightarrow E = eV$$

$$= \frac{3}{2}Nk_BT$$

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$$dS = \frac{3}{2} N k_B \frac{dT}{T} + N k_B \frac{dV}{V} \leftarrow \begin{array}{l} PV = nRT \\ P = \frac{N}{V} k_B T \end{array}$$

$$= N k_B \left(\frac{3}{2} \frac{dT}{T} + \frac{dV}{V} \right)$$

$$S - S_0 = N k_B \left(\frac{3}{2} \ln\left(\frac{T}{T_0}\right) + \ln\left(\frac{V}{V_0}\right) \right) \quad ; \; n = N/V$$

$$= N k_B \left(\frac{3}{2} \ln\left(\frac{T}{T_0}\right) - \ln\left(\frac{n}{n_0}\right) \right) \qquad \frac{n}{n_0} = \frac{V_0}{V}$$

$$\Rightarrow S = N k_B \left(\frac{3}{2} \ln(T) - \ln(n) + c_0(N) \right)$$

H - Function

$$f = \frac{n}{(2\pi k_B T)^{3/2}} e^{-\frac{c^2}{2RT}}$$

maxwellian

$$H = - \int_{\mathbb{R}^3} f \ln f$$

$$= - \int_{\mathbb{R}^3} f \left(\ln(n) - \frac{3}{2} \ln(2\pi k_B T) - \underbrace{\frac{c^2}{2RT}}_{= \frac{mc^2}{2Tk_B}} \right) dc \quad ; \; R = \frac{k_B}{m}$$

$$\Rightarrow \int \frac{m}{2} c^2 f \, dc = \frac{3}{2} n k_B T$$

normalisation of f $\quad \frac{1}{n} \int_{\mathbb{R}^3} f \, dc = 1$

$$\Rightarrow H = -n \ln(n) + \frac{3}{2} n \ln(T) + \frac{3}{2} \frac{k_B T}{k_B T} + c_1$$

$$= -n \left(\ln(n) - \frac{3}{2} \ln(T) \right) + \tilde{c}_1 \quad \text{note similarity with } S \text{ above?}$$

(.) Recall: $f \equiv f(c, t)$

$$\Rightarrow \frac{\partial f}{\partial t} = J(f, f) \quad \text{(Boltzmann eqn.)}$$

$$\rightarrow \frac{\partial H}{\partial t} = -\frac{\partial}{\partial t} \int_{\mathbb{R}^3} f \ln f \, dc$$

$$= - \int_{\mathbb{R}^3} \left(\frac{\partial f}{\partial t} \ln f + f \frac{1}{f} \frac{\partial f}{\partial t} \right) dc$$

$$= - \int_{\mathbb{R}^3} \frac{\partial f}{\partial t} (1 + \ln f) \, dc$$

$$= - \int_{\mathbb{R}^3} J(f, f) \ln f \, dc - \underbrace{\int_{\mathbb{R}^3} J(f, f) \, dc}_{0 \text{ (collisional invariants)}} = -I_\phi \quad ; \; \phi = \ln f(c)$$

$$\rightarrow \frac{\partial H}{\partial t} = -\int_{\mathbb{R}^3} \partial(f,f)\left(\ln(f(c)) + \ln(f(z)) - \ln(f(c')) - \ln(f(z'))\right) J(f,f)\, dc$$

$$= -\int_{\mathbb{R}^3} g(c,z)\underbrace{\left(f(c')f(z') - f(c)f(z)\right)}_{\circledast} \underbrace{\ln\left(\frac{f(c)f(z)}{f(c')f(z')}\right)}_{\star} dc\, dz\, dA_c$$

if $\circledast > 0$, $\star < 0$, ~~hold~~ here $\frac{\partial H}{\partial t} > 0$

if $\circledast < 0$, $\star > 0$, here $\frac{\partial H}{\partial t} > 0$

$\Big\}$ always larger than 0, $= 0$ iff $\circledast = 0$.

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$$\frac{dy}{dt} = \frac{\bar{y} - y}{\tau} \quad (\tau > 0)$$

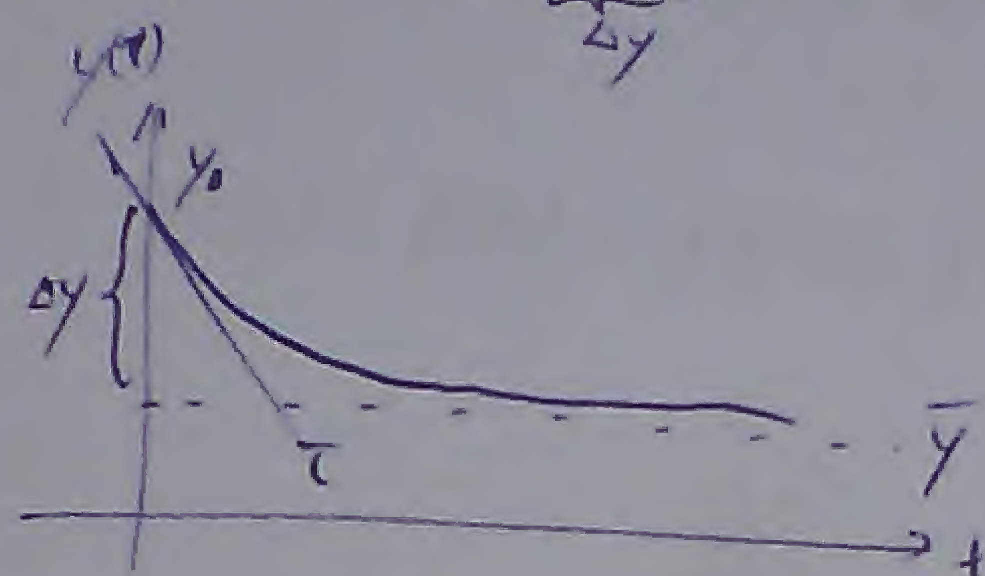
$$\int_{y_0}^{y} \frac{d\tilde{y}}{\bar{y} - \tilde{y}} = \int_0^t \frac{1}{\tau}\, d\tilde{t}$$

$$\rightarrow -\ln(\bar{y} - \tilde{y})\Big|_{y_0}^{y} = \frac{t}{\tau}$$

$$\rightarrow \ln\frac{\bar{y} - y}{\bar{y} - y_0} = \frac{-t}{\tau}$$

$$\Rightarrow \bar{y} - y = (\bar{y} - y_0)\, e^{-t/\tau}$$

$$y(t) := \bar{y} - \underbrace{(\bar{y} - y_0)}_{\Delta y} e^{-t/\tau}$$



The BGK Eqn:

Recall $\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$

BGK:

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{f^{(eq)} - f}{\tau}$$

Dimensional analysis:

Example: Compressible (steady) N-S eqn.

$$\frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}\left\{\mu\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\beta}{\partial x_\beta}\right)\right\}$$

dyn pressure $p + \frac{1}{2}\rho u^2 =$ const $\qquad \tau_{\alpha\beta}$

$$\tilde{\rho} = \frac{\rho}{\rho_\infty} \qquad \tilde{p} = \frac{p}{\rho_\infty u_\infty^2}$$

$$\tilde{u}_\alpha = \frac{u}{U_\infty} \qquad \tilde{x}_\alpha = \frac{x_\alpha}{L}$$

Dimensionless

$$\frac{\rho_\infty u_\infty^2}{L}\frac{\partial(\tilde{\rho}\tilde{u}_\alpha\tilde{u}_\beta)}{\partial\tilde{x}_\beta} + \frac{\rho_\infty u_\infty^2}{L}\frac{\partial\tilde{p}}{\partial\tilde{x}_\alpha} = \frac{\mu u_\infty}{L^2}\frac{\partial}{\partial\tilde{x}_\beta}\left(\frac{\partial\tilde{u}_\alpha}{\partial\tilde{x}_\beta} + \frac{\partial\tilde{u}_\beta}{\partial\tilde{x}_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial\tilde{u}_\beta}{\partial\tilde{x}_\beta}\right)$$

$$\Rightarrow \frac{\partial(\tilde{\rho}\tilde{u}_\alpha\tilde{u}_\beta)}{\partial\tilde{x}_\beta} + \frac{\partial\tilde{p}}{\partial\tilde{x}_\alpha} = \underbrace{\frac{\mu}{\rho_\infty u_\infty L}}_{\frac{1}{Re}}(\ldots)$$

Chapman – Enskog expansion

Recall : BGK Equation → Non-Dimensionalise

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{f^{(eq)} - f}{\tau} = (f^{(eq)} - f)\,\nu \quad ; \ \nu = \frac{1}{\tau}$$

$$\tilde{x}_\alpha = \frac{x_\alpha}{L} \qquad \tilde{t} = \frac{t}{L/\bar{c}} \qquad \frac{1}{n}\int f(c)\, dc \ , \ c = \{c_x, c_y, c_z\}$$

$$c_\alpha = \frac{c_\alpha}{\bar{c}} \ \text{average velocity} \qquad \tilde{f} = \frac{f\,\bar{c}^3}{n_0} \qquad f = \frac{n}{\bar{c}^3} \qquad \tilde{\nu} = \frac{\nu}{\nu_0} = \frac{\nu}{\bar{c}}\lambda$$

$$\Rightarrow \frac{n_0 \bar{c}}{\bar{c}^3 L}\frac{\partial \tilde{f}}{\partial \tilde{t}} + \bar{c}\,\frac{n_0}{\bar{c}^3}\tilde{c}_\alpha \frac{1}{L}\frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \frac{\bar{c}}{\lambda}\frac{n_0}{\bar{c}^3}\tilde{\nu}\,(\tilde{f}^{(eq)} - f)$$

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \underbrace{\frac{L}{\lambda}}_{\text{mfp}}\overset{\frac{1}{Kn}}{}\,\tilde{\nu}\,(\tilde{f}^{(eq)} - \tilde{f})$$

set $Kn \equiv \varepsilon$

As $\varepsilon \to 0$ $f \approx f^{(eq)}$

Assume $\varepsilon \ll 1$

$$f = \overset{f^{(eq)}}{f_0} + \varepsilon f_1 + \varepsilon^2 f_2 + \varepsilon^3 f_3 + \dots$$

$$= \sum_{k=0}^{\infty} \varepsilon^k f_k$$

Substitute in BGK

$$\varepsilon\,\frac{\partial(\tilde{f}_0 + \varepsilon\tilde{f}_1 + \varepsilon^2\tilde{f}_2 + \ )}{\partial t} + \varepsilon\,\tilde{c}_\alpha \frac{\partial(\tilde{f}_0 + \varepsilon\tilde{f}_1 + \varepsilon^2\tilde{f}_2 + \dots)}{\partial \tilde{x}_\alpha} = \tilde{\nu}\,(\tilde{f}^{(eq)} - \tilde{f}_0 - \varepsilon\tilde{f}_1 - \varepsilon^2\tilde{f}_2 - \dots)$$

ε^0: $\tilde{f}^{(eq)} = +\tilde{f}_0$

ε^1: $\dfrac{\partial \tilde{f}_0}{\partial t} + \tilde{c}_\alpha \dfrac{\partial \tilde{f}_0}{\partial \tilde{x}_\alpha} = -\tilde{\nu}\tilde{f}_1$

ε^k: $\dfrac{\partial \tilde{f}_{k-1}}{\partial t} + \tilde{c}_\alpha \dfrac{\partial \tilde{f}_{k-1}}{\partial \tilde{x}_\alpha} = -\tilde{\nu}\tilde{f}_k$

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BGK - eqn.

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \frac{1}{\varepsilon} \cdot \tilde{\upsilon}(\tilde{f}^{(eq)} - \tilde{f}) \quad (1)$$ non-dimensional form.

(non - dimensional form)

$\varepsilon = K_n = \frac{\lambda}{L}$ ← mean free path / ← char. length scale.

Note:

$$\int_{\mathbb{R}^3} \phi(c)(f^{(eq)} - f)\, d\underline{c} = 0 \qquad \phi(c) = \begin{cases} m \\ mc \\ \frac{1}{2}mc^2 \end{cases}$$

— e.g. $n = \int_{\mathbb{R}^3} f\, d\underline{c} = \int_{\mathbb{R}^3} f^{(eq)}\, d\underline{c}$

$n\underline{u} = \int_{\mathbb{R}^3} \underline{c} f\, d\underline{c} = \int_{\mathbb{R}^3} c f^{(eq)}\, d\underline{c}$

Perturbation around $f^{(eq)} \equiv f_0$

$$f = \sum_{k=0}^{\infty} \epsilon^k f_k$$

Substitute into BGK eqn:

$$\frac{\partial \tilde{f}_0}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}_0}{\partial \tilde{x}_\alpha} = -\tilde{\upsilon}\tilde{f}_1 \quad : \epsilon_1 \qquad (2)$$

$$\vdots$$

$$\frac{\partial \tilde{f}_k}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}_k}{\partial \tilde{x}_\alpha} = -\tilde{\upsilon}\tilde{f}_{k+1} \quad : \epsilon_{k+1} \;;\; \epsilon \equiv \varepsilon \equiv K_n$$

Consider (2) in dimensional form:

$$\underbrace{\frac{\partial f_0}{\partial t} + c_\alpha \frac{\partial f_0}{\partial x_\alpha}}_{\frac{Df_0}{Dt}} = -\varepsilon \upsilon f_1 \quad (3)$$

$$\boxed{|c-u|^2 = \xi^2 = \xi_1^2 + \xi_2^2 + \xi_3^2}$$

Recall:

$$f_0 = \frac{n(x,t)}{(2\pi RT)^{3/2}} e^{\frac{-|c-u|^2}{2RT}} \qquad (f = n\hat{f})$$

$$\frac{Df_0}{Dt} = \hat{f}_0 \frac{Dn}{Dt} + n\frac{D\hat{f}_0}{Dt}$$

$$= \hat{f}_0 \frac{Dn}{Dt} + n\left(\frac{\partial \hat{f}_0}{\partial T}\frac{DT}{Dt} + \frac{\partial \hat{f}_0}{\partial u_\alpha}\frac{Du_\alpha}{Dt}\right)$$

$$\frac{\partial \hat{f}}{\partial u_\alpha} = \hat{f}_0\left(\frac{\xi^2}{2RT^2} - \frac{3}{2T}\right) = \hat{f}_0\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right)\frac{1}{T}$$

$$(3) \Rightarrow \varepsilon \upsilon f_1 = -\hat{f}_0 \left\{ \frac{Dn}{Dt} + n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right) \underbrace{\frac{1}{T}\frac{DT}{Dt}}_{\frac{D\ln T}{Dt}} + n\frac{\xi_\alpha}{RT}\frac{Du_\alpha}{Dt} \right\}$$

Consider Moment Relations:

$$(i)\ \frac{\partial n}{\partial t} + \frac{\partial (n u_\alpha)}{\partial x_\alpha} = 0$$

$$\Longleftrightarrow \frac{\partial n}{\partial t} + u_\alpha \frac{\partial n}{\partial x_\alpha} = -n\frac{\partial u_\alpha}{\partial x_\alpha}$$

$$(ii)\ \frac{\partial (n u_\alpha)}{\partial t} + \frac{\partial (n u_\alpha u_\beta)}{\partial x_\beta} + \frac{1}{m}\frac{\partial P_{\alpha\beta}}{\partial x_\beta} = 0$$

$$\Longleftrightarrow u_\alpha\left(\frac{\partial n}{\partial t} + \frac{\partial n u_\beta}{\partial x_\beta}\right) + n\left(\frac{\partial u_\alpha}{\partial t} + \frac{\partial u_\alpha}{\partial x_\beta}\right)$$

$$+ \frac{1}{m}\frac{\partial}{\partial x_\beta}\underbrace{\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \left(f_0 + \underbrace{\varepsilon f_1 + \dots}_{\text{higher order term}}\right) d\xi}_{p\delta_{\alpha\beta}} = 0$$

$$(i)\ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_\alpha)}{\partial x_\alpha} = 0$$

$$(ii)\ \frac{\partial (\rho u_\alpha)}{\partial t} + \frac{\partial (\rho u_\alpha u_\beta)}{\partial x_\beta} + \frac{\partial P_{\alpha\beta}}{\partial x_\beta} = 0$$

$$(iii)\ \frac{\partial E}{\partial t} + \frac{\partial E u_\beta}{\partial x_\beta} + \frac{\partial P_{\alpha\beta} u_\beta}{\partial x_\beta} + \frac{\partial q_\beta}{\partial x_\beta} = 0$$

$$P_{\alpha\beta} = m\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta f\, d\xi$$

$$(iii)\ \frac{\partial T}{\partial t} + u_\beta \frac{\partial T}{\partial x_\beta} = -\frac{2}{3}T\frac{\partial u_\beta}{\partial x_\beta}$$

$$\Longleftrightarrow \frac{\partial \ln T}{\partial t} + u_\beta \frac{\partial \ln T}{\partial x_\beta} = -\frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta}$$

$$\Longleftrightarrow \varepsilon \upsilon f_1 = -\hat{f}_0 \left\{ -n\frac{\partial u_\beta}{\partial x_\beta} + \xi_\beta \frac{\partial n}{\partial x_\beta} + n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right)\left(\xi_\beta \frac{\partial \ln T}{\partial x_\beta} - \frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta}\right)\right.$$

$$\left. + n\frac{\xi_\alpha}{RT}\left(\xi_\beta \frac{\partial u_\alpha}{\partial x_\beta} - \frac{1}{\rho}\frac{\partial p}{\partial \alpha}\right)\right\}$$

$$= -\hat{f}_0\left\{\xi_\beta \frac{\partial n}{\partial x_\beta} + \underbrace{n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right)\xi_\beta \frac{\partial \ln T}{\partial x_\beta}}_{(a)} - n\frac{\xi^2}{3RT}\frac{\partial u_\beta}{\partial x_\beta} + n\frac{\xi_\alpha}{RT}\left(\xi\frac{\partial u_\alpha}{\partial x_\beta} - \frac{1}{\rho}\frac{\partial p}{\partial \alpha}\right)\right\}\ ⊛$$

Use ideal gas:

$$\frac{\partial n}{\partial x_\beta} = \frac{\partial}{\partial x_\beta}\left(\frac{p}{k_B T}\right)$$

$$= \frac{1}{k_B T}\frac{\partial p}{\partial x_\beta} - \frac{p}{k_B T^2}\frac{\partial T}{\partial x_\beta} \qquad p = \rho RT = n k_B T \Rightarrow \frac{1}{k_B T} = \frac{n}{\rho RT}$$

$$= \underbrace{\frac{n}{\rho RT}\frac{\partial p}{\partial x_\beta}}_{⊛} - \underbrace{\overset{=n}{\frac{p}{k_B T}}\frac{\partial \ln T}{\partial x_\beta}}_{(b)}$$

$$\varepsilon \upsilon f_1 = -\hat{f}_0\left\{\overset{(a)+(b)}{n\left(\frac{\xi^2}{2RT} - \frac{5}{2}\right)}\xi_\beta \frac{\partial \ln T}{\partial x_\beta} + \frac{n}{RT}\left(\xi_\alpha \xi_\beta - \frac{1}{3}\delta_{\alpha\beta}\xi^2\right)\frac{\partial u_\alpha}{\partial x_\beta}\right\}$$

Now let,

$$f = f_0 + \varepsilon f_1$$

$$P_{\alpha\beta} = m \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta (f_0 + \varepsilon f_1) d\xi$$

$$= P\delta_{\alpha\beta} - \frac{\rho}{\nu} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \hat{f}_0 \left(\left(\frac{\xi^2}{2RT} - \frac{5}{2}\right) \xi_\gamma \frac{\partial \ln T}{\partial x_\gamma} + \frac{1}{RT}\left(\xi_\gamma \xi_\sigma - \frac{1}{3}\delta_{\gamma\sigma}\xi^2\right)\frac{\partial u_\gamma}{\partial x_\sigma} \right)$$

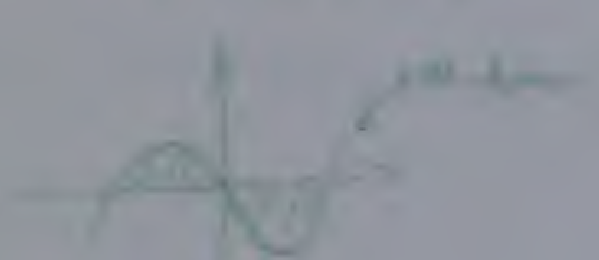
Consider:

$$\int_{\mathbb{R}^3} \xi_1^l \xi_2^m \xi_3^n \hat{f}_0 \, d\xi$$

+ permutations

=0 if any l, m, n is odd

due to symmetry, if function odd (ξ_1, ξ_2, ξ_3), integral is zero



Consider:

$\alpha \neq \beta$

$$P_{\alpha\beta} = \frac{-\rho}{\nu RT} \frac{\partial u_\gamma}{\partial x_\sigma} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \xi_\gamma \xi_\sigma \hat{f}_0 \, d\xi$$

non only if $\alpha = \gamma, \beta = \sigma$ — $\alpha = \sigma, \beta = \gamma$

$$= \frac{-\rho}{\nu RT}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right) \underbrace{\int_{\mathbb{R}^3} \hat{f}_0 \xi_\alpha^2 \xi_\beta^2 \, d\xi}_{(RT)^2}$$

$$= \frac{-\rho RT}{\nu}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right)$$

Consider:

$\alpha = \beta$

$$P_{\alpha\beta} = P - \frac{\rho}{\nu RT} \int_{\mathbb{R}^3} \hat{f}_0 \xi_\alpha^2 \left(\xi_\gamma \xi_\sigma - \frac{1}{3}\delta_{\gamma\sigma}\xi^2\right) \frac{\partial u_\gamma}{\partial x_\sigma} d\xi$$

$$= P - \frac{\rho RT}{\nu}\left(2\frac{\partial u_\alpha}{\partial x_\alpha} - \frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta}\right)$$

no summation

$$P_{\alpha\beta} = P\delta_{\alpha\beta} - \frac{\rho}{\nu RT}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\gamma}{\partial x_\gamma}\right)$$

Heat flux

$$q_\beta = \frac{m}{2}\int_{\mathbb{R}^3} \xi_\beta \xi^2 (f_0 + \varepsilon f_1) d\xi = \underbrace{\frac{5}{2}R}_{c_p} \underbrace{\frac{\rho}{\nu}}_{\mu} \frac{\partial T}{\partial x_\beta}$$

issues of BGK model

If we set ν to properly recover viscosity, BGK enforces the heat conduction coefficient; these two are not independent of each other

also, $Pr = \frac{c_p \mu}{\kappa} = 1$ for BGK model

must know the steps! will be in exam!

LBM 25th Nov 2016

Ch. 8. Lattice Gas Automata

So far: kinetic theory

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \begin{cases} J(f,f) & \text{Boltzmann} \\ \frac{1}{\tau}(f^{(eq)} - f) & \text{BGK} \end{cases}$$

$c = (c_\alpha)_{\alpha=1,2,3} \in \mathbb{R}^3$

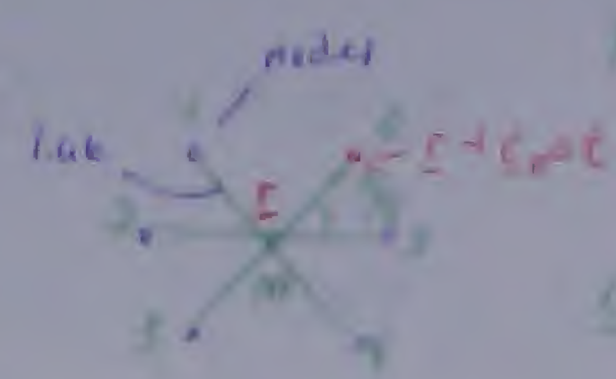
2D Boltzmann $\underline{c} = \begin{pmatrix} c\cos\phi \\ c\sin\phi \end{pmatrix}$

$c \in [0, \infty)$

$\phi \in [0, 2\pi)$

(8.1) lattice-gas model

Idea: Restrict $|\underline{c}| = c$ to one value $c \equiv c_{ref}$ and six angles ϕ



$\underline{c} = c(\cos(\frac{\pi}{3}k), \sin(\frac{\pi}{3}k))$, $k = 0, \ldots, 5$

Let Δt be fixed. Assume, we simulate gas by taking "snapshots" at time instances $\Delta t\, n$; $n \in \mathbb{N}$

Assume non-dimensional variables:

$$\tilde{c} = \frac{c}{c_{ref}} = 1$$

$$\tilde{m} = \frac{m}{m_{ref}}$$

$$\tilde{t} = \frac{t}{\Delta t} \Rightarrow \Delta\tilde{t} = 1$$

$$|c\Delta t| = 1$$

Simulate Lattice-gas

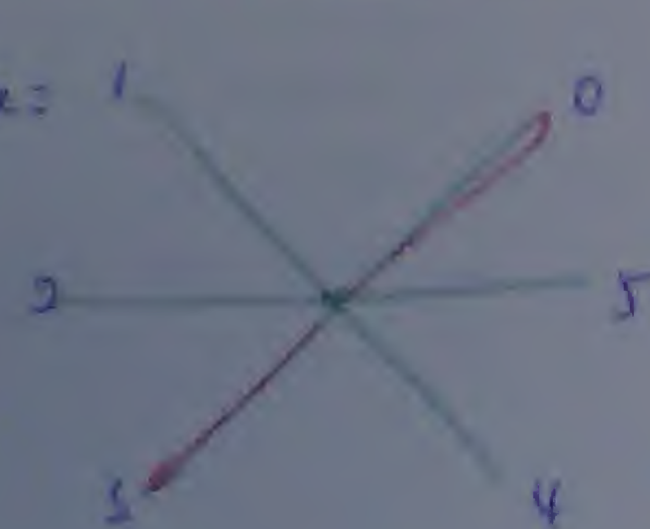
Need Model:

1. "Lattice Configuration"

At each nodes $\underline{r}$ there can only be one particle having velocity c_k "exclusion principle"

$\Rightarrow$ can encode the state at node $\underline{r}$ (at time t) using 6-bit binary number.

Example:



$\Rightarrow (0\,0\,1\,0\,0\,1) = n(\underline{r}, t)$

there are total of $2^6 = 64$ possible states at a given time.

(ii) "Evolution"

Two-step operator.

"Collision" (0, 1) could be zero or 1 at node.

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t) \; ; \; i = 0, \ldots, 5$$

"Streaming" → recall, $\underline{c}_i = (\cos(\frac{\pi}{3}i), \sin(\frac{\pi}{3}i))$ $c = 1$

$$n_i(\underline{r}+\underline{c}_i, t+1) = n_i'(\underline{r},t)$$

Collision Model

Define "collision" is a mapping $\Delta_i : \{0,1\} \to \{0,1\}$

$$n_i(\underline{r},t) \mapsto n_i'(\underline{r},t)$$

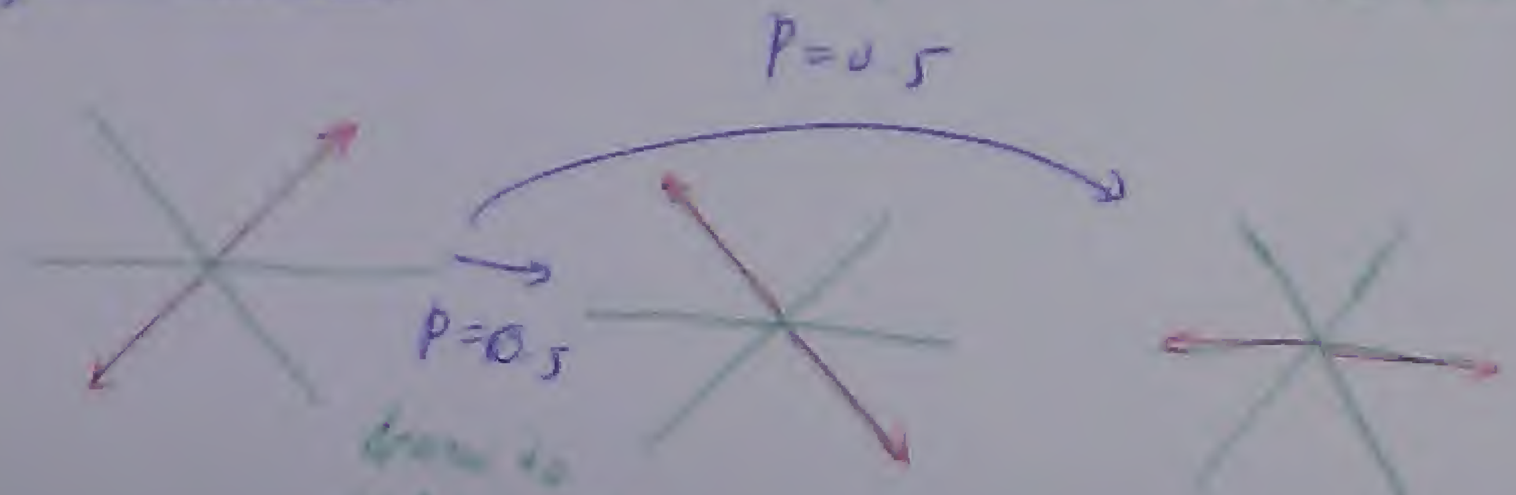
need conservation

mass: $\sum_{i=0}^{5} n_i'(\underline{r},t) = \sum_{i=0}^{5} n_i(\underline{r},t) \; ; \; \forall \underline{r}, t$

momentum: $\sum_{i=0}^{5} n_i' c_i = \sum_{i=0}^{5} n_i c_i$

Energy: $\sum_{i=0}^{5} n_i c^2 = \sum_{i=0}^{5} n_i' c^2$ since there is only 1 possible c_i (not 0) → holds from mass & momentum conservation, automatically

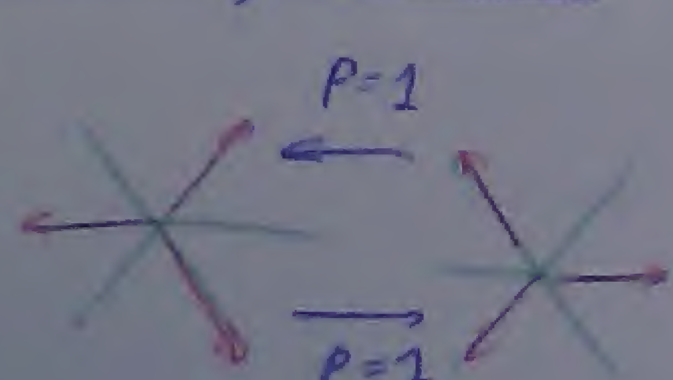
(i) Binary Collision (each collision experienced at a node must conserve mass & momentum!)



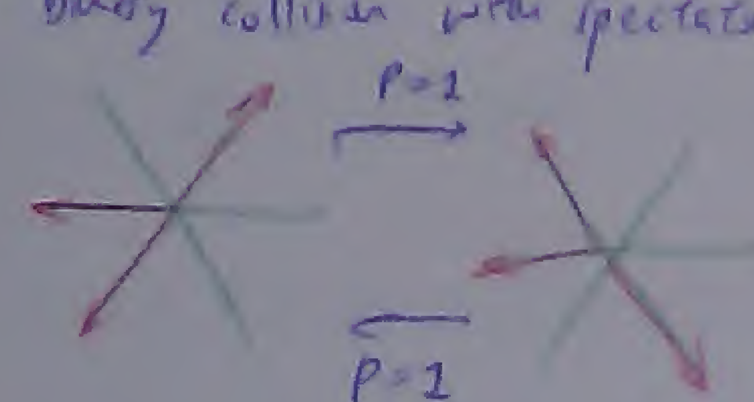
tends to evolve to this state after collision and vice-versa.

(ii) three-way collision

(a)



(b) "binary collision with spectator"



(iii) Four-way collision

→ exclude trivial collision that is e.g. six-way collision.

→ in other words, if the configuration doesn't change, we don't consider it. (trivial collision)

(8.3) Analysis of the LGA

(8.3.1) The Collision Operator:

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t) \quad ; \quad \Delta_i \in \{-1, 0, 1\}$$

Remark: In the following

$$\overline{i+k} = \begin{cases} i+k & \text{if } i+k < 6 \\ i+k-6 & \text{if } i+k \geq 6 \end{cases} \qquad i,k = 0,\dots,5$$

essentially, this is a mod operator
in C programming $\Rightarrow$ $i \% 6$ [illegible]

Derive an algebraic Expression for Δ_i

Then $\Delta = (\Delta_i)_{i=0,\dots,5}$

Consider Binary collision (Type (A))

Case	n_i	n_{i+1}	n_{i+2}	n_{i+3}	n_{i+4}	n_{i+5}
1	1	0	0	1	0	0
2	0	1	0	0	1	0
3	0	0	1	0	0	1

$$\delta_i^{(A,1)} = n_i n_{i+3} (1-n_{i+1})(1-n_{i+2})(1-n_{i+4})(1-n_{i+5})$$

$$\delta_i^{(A,2)} = n_{i+1} n_{i+4} (1-n_i)(1-n_{i+2})(1-n_{i+3})(1-n_{i+5})$$

$$\delta_i^{(A,3)} = \dots$$

Collision operator is constructed:

$$\Delta_i^{(A)} = a_1 \delta_i^{(A,1)} + a_2 \delta^{(A,2)} + a_3 \delta^{(A,3)}$$

$$a_1 = -1 \quad a_2 = \xi \; ; \; \xi = \{0,1\} \quad a_3 = 1-\xi.$$

"random bit"

$$\Rightarrow \Delta_i^{(A)} = -\delta_i^{(A,1)} + \xi \delta_i^{(A,2)} + (1-\xi)\delta_i^{(A,3)}$$

If binary case 1 of binary collision is detected, we know that after collision, n_i will be zero definitely. Hence the Δ_i must be -1 on n_i

Done similarly for 3-way collision:

$$\delta_i^{(B,1)} = n_i n_{i+2} n_{i+4} (1-n_{i+1})(1-n_{i+3})(1-n_{i+5})$$

$$\delta_i^{(B,2)} = n_{i+1} n_{i+3} n_{i+5} (1-n_i)(1-n_{i+2})(1-n_{i+4})$$

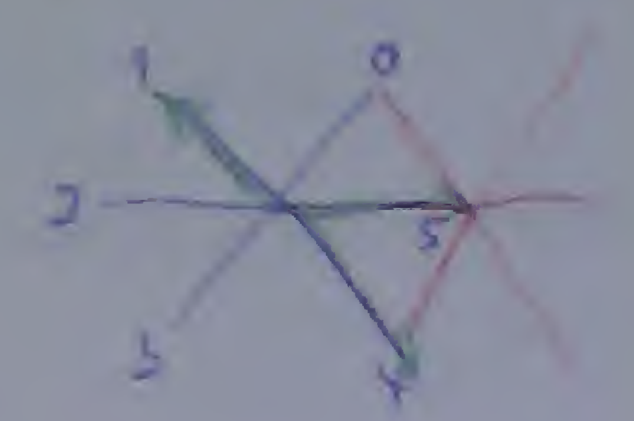
$$\Delta_i^{(B)} = -\delta_i^{(B,1)} + \delta_i^{(B,2)}$$

$$\Rightarrow \underbrace{\Delta_i = A_i^{(A)} + \Delta_i^{(B)}}$$

allowed because if it is case [illegible], either (A) is up or (B) is up [illegible]

Implementation of LGA 1/12/2016

① Particles



$n = (110010)$

⊛ In practice: use 8 bit number

⊛ Possible datatypes

C: unsigned char
(int8_t (C99))

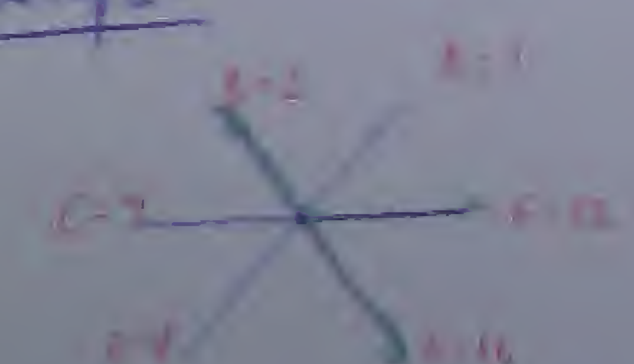
MATLAB: uint8

FORTRAN: INTEGER(1)
(90+)

Algebraic vs. "Logical" method

i.e. Integer arithmetic or boolean operators

Example:



$n = (110010)$

$= 1\cdot\underbrace{2^5}_{32} + 1\cdot\underbrace{2^4}_{16} + 1\cdot\underbrace{2^1}_{2}$

$= (50)_{10}$

Starting directly → A=(000001)₂, B=(000010)=2, C=(000100)=4

Set here as

$n = B + E + F$
$= (50)_{10}$ } ① algebraic way

or: (in C programming) binary operator (000001) or (000010)

$n = \underbrace{(1 \ll 1)}_{B} \mid \underbrace{(1 \ll 4)}_{E} \mid \underbrace{(1 \ll 5)}_{F};$

⇒ (000010) = B
or (010000) = E
or (100000) = F

$(110010)_2 = (50)_{10}$

$\boxed{\text{Initialization}}$

Start with

$\frac{1}{6}\sum_{i=0}^{5} N_i =: \rho \quad \rho \in [0,1]$

average Eq.?

① algebraic method

for $\rho = \rho_0 \in [0,1]$; $n = (n_5, \dots n_0)$

```
for i = 1, ..., N_x        # nodes
    n(r_i, t=0) = 0
    for k = 0, ..., 5
        if [rand + ρ0]        (random number, float division 1.1 => 1)
            n_k(r_i, t=0) += C_k
        end if
    end for
end for
```

A = C_0
B = C_1
C = C_2

bit "OR"

(001001)
+ (100000)
(101001)

② boolean method

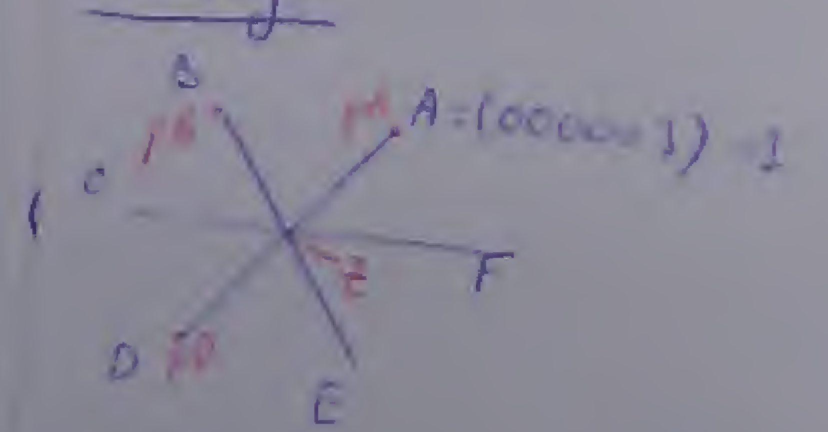
```
for i = 1, ..., N_x
    n(r_i, t=0) = 0
    for k = 0, ..., 5
        if [rand + ρ0] (=1)
            n_k(r_i, t=0) |= (1 << k)
        end if
    end for
end for
```

Collision: implemented using lookup table.

Index: B	Index: ξ	Index: state (6 bit)	value	
0	0	000000	(0 0) 000000	
0	0	000001	000001	
0	0	000010	000010	
		⋮	⋮	
0	0	001001	010010	9th entry
		⋮	⋮	
		010101	101010	21st entry
		⋮		
		111111	111111	63rd entry
0	1	000000	000000	64th entry
		⋮	⋮	
1		001001	100100	
1		111111	111111	
1	0	000000		

B: bit is for boundary conditions
ξ = bit is the random 1 | 0.

Streaming



Def let pA be neighbour in "direction A"

$n(pA) \mathrel{|}= (n'(z) \,\&\, A)$: $n'(z)$ is state after collision. it checks whether particle occupies A after collision

$n(pB) \mathrel{|}= (n'(z) \,\&\, B)$

B(000010)

n' = (0 1 0 1 1 0)

LBM 8th Dec

Recall:

Maxwell-B

$f(s) =$

$\Rightarrow \frac{\partial f}{\partial t}$

$P(C \in$

LGA

LBM 2nd Dec 2016

(1)

LGA analysis

The collision operator

~~...~~

$$\Delta_i(n) = n_i'(n) - n_i$$

$$n = (n_5\, n_4\, n_3\, n_2\, n_1\, n_0)$$

Recall:

$$n_0 n_3 (1-n_1)(1-n_2)(1-n_4)(1-n_5) = \begin{cases} 1 & \text{if } n = (001001) \\ 0 & \text{otherwise} \end{cases}$$

(001001)

Generalized Expression for identifying a state:

First, define set

$$S = \{0,1\}^6 = \{0,1\} \times \{0,1\} \times \{0,1\} \times \dots \times \{0,1\}$$
$$= \{ (s_5 \dots s_0) ; s_i \in \{0,1\},\ i = 0, \dots, 5 \} \quad \# S = 64$$

Now note: For $n_j, s_j \in \{0,1\}$

$$n_j^{s_j} (1-n_j)^{1-s_j} = \begin{cases} 1 & \text{if } n_j = s_j \\ 0 & \text{if } n_j \neq s_j \end{cases}$$

Check

$$n_j = 0 : \begin{cases} s_j = 0 : & 0^0 \cdot 1^1 = 1 \\ s_j = 1 : & 0^1 \cdot 1^0 = 0 \end{cases}$$

Similar for $n_j = 1$.

$\Rightarrow$ Define "Algebraic" Kronecker Delta:

$$\delta_{n,s} = \prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j} = \begin{cases} 1, & n = s \\ 0, & n \neq s \end{cases}$$

Transition bit:

For each $s, s' \in S$ "transition bit"

$$\xi_{s,s'} = \begin{cases} 1 & s' \longrightarrow s \text{ connected by admissible collision} \\ 0 & \text{otherwise} \end{cases}$$

(1) (i, i)

Note: This will be set such that $\langle \xi_{s,s'} \rangle$ is the correct probability for transition between s & s'.
(expectation value of ~~transition~~ probability)

Note:

$$\sum_{s' \in \mathcal{S}} \langle \xi_{s,s'} \rangle = 1$$

$$\sum_{s' \in \mathcal{S}} \xi_{s,s'} = 1$$ still 1 because at a given time, there can be only one result of transition.

Function $\Delta_i(n) = n_i'(n) - n_i$

given input state n, output state is

$$n_i'(n) = \sum_{s \in \mathcal{S}} \sum_{s' \in \mathcal{S}} s_i' \xi_{s,s'} \underbrace{\prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}}_{\delta_{n,s}}$$

only one for s is the ...

$$n_i = \sum_{s \in \mathcal{S}} s_i \delta_{n,s}$$

$$= \sum_{s'} \sum_{s} s_i \delta_{n,s} \xi_{s,s'}$$

$$\Delta_i(n) = \sum_{s,s' \in \mathcal{S}} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}$$

	Kinetic Theory	Lattice Methods
microdynamics	Eqn of motion for each particle	LGA
Stochastic description	→ Distribution function. $f(c, x, t)$ → Equilibrium (maxwell-boltzmann)	
	For non equilibrium: Boltzmann Equation.	"averaged" LGA → Lattice Boltzmann Method.
Conservation Laws	→ moments + Chapman - Enskog	(discrete) Moments + Multiscale Expansion. check back on N-S eqn derivation

Equilibrium Solution of LGA

Postulate N_i: Probability of ~~the~~ link i being occupied.

Define: $\rho = \sum_{i=0}^{5} N_i$ $\quad$ $P(n_i = 1)$ $\quad$ $n = \int f \, dv$ only discrete momentum space. $\quad$ $\underline{u} = \frac{1}{\rho} \sum_{i=0}^{5} \underline{c}_i N_i$

statistically independent:

$N_i N_j$: probability $P(n_i = 1 \,\&\, n_j = 1)$

LBM 8th

Recall: Consider:

Maxwell- $P(n=(1\,1\,1\,1\,1\,1)) = \prod_{j=0}^{5} N_j$

$f(s) =$ $P(n=(0\,0\,0\,0\,0\,0)) = \prod_{j=0}^{5} (1-N_j)$

$\Rightarrow \frac{\partial f}{\partial t}$ $P(n=(1\,1\,1\,0\,0\,0)) = \prod_{j=0}^{2} (1-N_j) \prod_{j=3}^{5} N_j$

$p(C\in$ $$p(s) = \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$
$(s \in S)$

since N_j is invariant under collisions, hence conservation

$$p(s') = \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'}$$

$$= \sum_{s\in S} \langle \xi_{s,s'} \rangle \, p(s)$$

$\sum$ over all possible outcomes, $\{0,1\}$

LGA

$$= \sum_{s\in S} \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

$$\Rightarrow \sum_{s'\in S} s_i' \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'} = \sum_{s',s\in S} s_i' \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

since $\sum_{s\in S} \langle \xi_{s,s'} \rangle = 1$, multiply to LHS, then move the terms to LHS:

$$\sum_{s,s'\in S} (s_i'-s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j} = 0$$

$$\Rightarrow \underbrace{\prod_{j=0}^{5} (1-N_j)}_{\text{assume} \neq 0} \underbrace{\left(\sum_{s,s'\in S} (s_i'-s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} \Big(\underbrace{\frac{N_j}{1-N_j}}_{\eta_j} \Big)^{s_j} \right)}_{=0} = 0$$

multiply $\sum_{i=0}^{5} \log \eta_i$

$$\Rightarrow \sum_{i=0}^{5} \log \eta_i \sum_{s,s'\in S} (s_i'-s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} \eta_j^{s_j} = 0$$

$$= \sum_{s,s'\in S} \langle \xi_{s,s'} \rangle \left(\sum_{i=0}^{5} (s_i'-s_i) \log \eta_i \right) \prod_{j=0}^{5} \eta_j^{s_j} = 0$$

$$= \sum_{s,s'\in S} \langle \xi_{s,s'} \rangle \log\left(\frac{\prod \eta_i^{s_i'}}{\prod \eta_i^{s_i}} \right) \underbrace{\prod_{j=0}^{5} \eta_j^{s_j}}_{x_s} = 0$$

$$\Rightarrow \sum_{s,s'\in S} \langle \xi_{s,s'} \rangle \log\left(\frac{x_{s'}}{x_s} \right) x_s = 0 \qquad (1)$$

Note:

$$\sum_{s,s' \in S} x_s \langle \xi_{s,s'} \rangle = \sum_s x_s \underbrace{\sum_{s'} \langle \xi_{s,s'} \rangle}_{1}$$

$$= \sum_s x_s$$

$$= \sum_{s'} x_{s'} \underbrace{\sum_{s} \langle \xi_{s,s'} \rangle}_{\text{not necessarily 1 now but assume it } = 1}$$ note the difference $\sum_s \langle \xi_{s,s'} \rangle$ vs $\sum_{s'} \langle \xi_{s,s'} \rangle$

$$= \sum_{s,s'} x_{s'} \langle \xi_{s,s'} \rangle$$

$$\Rightarrow \sum_{s,s'} (x_s - x_{s'}) \langle \xi_{s,s'} \rangle = 0 \qquad (2)$$

$$-((1) + (2)) = 0$$

$$\sum_{s,s'} \underbrace{\left(-x_s \log\left(\frac{x_{s'}}{x_s}\right) + x_{s'} - x_s \right)}_{\geq 0} \underbrace{\langle \xi_{s,s'} \rangle}_{\geq 0} = 0 \qquad ⊛$$

$$\Updownarrow$$

$$\int_{x_{s'}}^{x_s} \log\left(\frac{t}{x_{s'}}\right) dt \geq 0$$

Case 1 $\langle \xi_{s,s'} \rangle = 0$ transition is allowed!

Case 2 $\langle \xi_{s,s'} \rangle \neq 0$ transition allowed!

(i) $s = s' \Rightarrow 0$

(ii) $x_s = x_{s'}$ $(s' \neq s)$ ⊛ will have non-trivial zero solution!

$$\Rightarrow \prod_{i=0}^{5} \eta_i^{s_i} = \prod_{i=0}^{5} \eta_i^{s'_i}$$

take log: $\sum_{i=0}^{5} (s'_i - s_i) \log \eta_i = 0.$

Satisfied if $\log \eta_i = -(a + \underline{b} \cdot \underline{c}_i)$

$$\Rightarrow \eta_i = e^{-(a + \underline{b} \cdot \underline{c}_i)} = \frac{N_i}{1 - N_i}$$

$$\rightarrow 1 - N_i = N_i e^{a + \underline{b} \cdot \underline{c}_i}$$

$$1 = N_i (1 + e^{a + \underline{b} \cdot \underline{c}_i})$$

$$N_i = \frac{1}{(1 + e^{a + \underline{b} \cdot \underline{c}_i})}$$

LBM 8th Dec 2016

Recall:

①

Maxwell-Boltzmann

$$f(\underline{c}) = A e^{-\beta^2 |\underline{c} - \underline{\alpha}|^2}$$

$$\Rightarrow \frac{\partial f}{\partial t}\Big|_{collision} = 0$$

$$P(\underline{c} \in V_c) = \frac{1}{n} \int_{V_c} f(\underline{c})\, d\underline{c}$$

the moments

$$n = \int_{\mathbb{R}^3} f(\underline{c})\, d\underline{c}$$

$$n\underline{u} = \int_{\mathbb{R}^3} \underline{c}\, f(\underline{c})\, d\underline{c}$$

$$\frac{3}{2} k_B T = \frac{m}{2} \int_{\mathbb{R}^3} \underbrace{|\underline{c} - \underline{u}|^2}_{\xi} f(\underline{c})\, d\underline{c}$$

can express $A, \beta, \underline{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ as function of $n, T, \underline{u} = (u_1, u_2, u_3)$

LGA

set ~~...~~ $n_i(\underline{r} + \underline{c}_i, t+1) = n_i(\underline{r}, t) + \Delta_i(\underline{r}, t)$

admits an equilibrium s.t. $\langle \Delta_i \rangle = 0$

(1) $\langle n_i \rangle = N_i^{(eq)} = \dfrac{1}{1 + e^{a + \underline{b} \cdot \underline{c}_i}}, \quad i = 0, \dots, 5.$

(2) $\rho = \sum_{i=0}^{5} N_i^{(eq)}$

(3) $\rho \underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i^{(eq)}$

cannot express a, $\underline{b} = (b_1, b_2)$ as functions of $\rho, \underline{u} = (u_1, u_2)$

③ Preliminary steps:

Let $\underline{u} = (u_\alpha)_{\alpha = 1,2}$

Let $a = a(\rho, \underline{u})$

$\underline{b} = \underline{b}(\rho, \underline{u})$

small velocity approximation

$$a(\rho, u) = \underbrace{a(\rho, 0)}_{a_0(\rho)} + \underbrace{\frac{\partial a}{\partial u_\alpha}\Big|_{(\rho,0)}}_{a_{1,\alpha}(\rho)} u_\alpha + \underbrace{\frac{1}{2} \frac{\partial a}{\partial u_\alpha \partial u_\beta}\Big|_{(\rho,0)}}_{a_{2,\alpha\beta}} u_\alpha u_\beta + \dots$$

$\Rightarrow a = a_0(\rho) + a_{1,\alpha} u_\alpha + a_{2,\alpha\beta} u_\alpha u_\beta + \dots$

$b_\alpha = b_{0,\alpha}(\rho) + b_{1,\alpha\beta} u_\beta + b_{2,\alpha\beta\gamma} u_\beta u_\gamma + \dots$

Constraints: will shape the final $N_i^{(q)}$

① At $\underline{u} = 0 \Rightarrow N_i = \text{const} \ \forall i$

$\Rightarrow b_{0,\alpha} = 0 \quad \alpha = 1,2$

② Symmetry: N_i should be invariant under

(i) coordinate reflection

ie $x \mapsto -x$

($u \mapsto -u \quad c_i \longrightarrow -c_i$)

$\Rightarrow a$ symmetric in $\underline{u}$,
b antisymmetric in $\underline{u}$

$\frac{1}{1+e^{a+b\cdot\xi_i}}$ } if this is invariant under reflection,
$a \to a$
$b\cdot c_i \to b\cdot(-c_i)$; ξ_i is symmetric, b antisym
will = to preserve N_i

$\Rightarrow a_{1,\alpha} = 0 \quad \alpha = 1,2$

$b_{2,\alpha\beta\gamma} = 0 \quad \alpha,\beta,\gamma = 1,2$

(ii) isotropy:

$b_{1,\alpha\beta} = b_1 \delta_{\alpha\beta}$

$a_{2,\alpha\beta} = a_2 \delta_{\alpha\beta}$

$\Rightarrow a = a_0(\rho) + a_2(\rho) u^2$

$b = b_{1,\alpha} u_\alpha$

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Substitute (1) ($N_i^{(eq)}$)   LBM 8th Dec 2016   (3)

$$N_i^{(eq)} = \frac{1}{1+e^{g_i(\rho,u)}} \; ; \; g_i = a_0(\rho) + a_2(\rho) u^2 + b_\alpha \underbrace{u_\alpha c_{i\alpha}}_{u\cdot c_i}$$

(2) Expand $N_i^{(eq)}$ in u

$$N_i^{(eq)} = \underset{(a)}{N_i^{(eq)}(\rho,0)} + \underset{(b)}{\frac{\partial N_i^{(eq)}}{\partial u_\alpha}\Big|_{u=0}} u_\alpha + \frac{1}{2} \underset{(c)}{\frac{\partial^2 N_i^{(eq)}}{\partial u_\alpha \partial u_\beta}\Big|_{u=0}} u_\alpha u_\beta + O(u^3)$$

(a) $N_i^{(eq)}(\rho,0) = \frac{1}{1+e^{g(\rho,0)}} = \frac{1}{1+e^{a_0}} = \frac{\rho}{6} =: d$; $\rho = \sum_{i=0}^{6} N_i^{(eq)}$

(b) $\underset{(i)}{(N_i^{(eq)})'} \underset{(iii)}{\frac{\partial g_i}{\partial u_\alpha}}$ $(N_i^{(eq)})' = \left(\frac{1}{1+e^x}\right)'\Big|_{x=a_0}$

chain derivation!

(c) $\underset{(ii)}{(N_i^{(eq)})''} \frac{\partial g_i}{\partial u_\alpha} \frac{\partial g_i}{\partial u_\beta} + (N_i^{(eq)})' \underset{(iv)}{\frac{\partial^2 g_i}{\partial u_\alpha \partial u_\beta}}$

(i) $(N_i^{(eq)})'\Big|_{u=0} = \frac{-e^{a_0}}{(1+e^{a_0})^2} = -\frac{1-d}{d} d^2 = d(d-1)$

(ii) $(N_i^{(eq)})''\Big|_{u=0} = \frac{e^{a_0}(e^{a_0}-1)}{(1+e^{a_0})^3} = \frac{1-d}{d} \cdot \frac{1-2d}{d} d^3 = d(d-1)(2d-1)$

(iii) $\frac{\partial g_i}{\partial u_\alpha}\Big|_{u=0} = b_1 c_{i,\alpha}$

(iv) $\frac{\partial^2 g_i}{\partial u_\alpha \partial u_\beta}\Big|_{u=0} = 2a_2 \delta_{\alpha\beta}$

$$N_i^{(eq)} = d + d(d-1) b_1 c_{i\alpha} u_\alpha + \frac{1}{2} d(d-1)(2d-1) b_1^2 c_{i\alpha} c_{i\beta} u_\alpha u_\beta + \frac{1}{2} d(d-1) 2a_2 \delta_{\alpha\beta} u_\alpha u_\beta$$

$$\Rightarrow N_i^{(eq)} = \underbrace{d}_{N_i^{(eq)}(\rho,0)} + \underbrace{d(d-1) b_1 c_{i,\alpha}}_{\frac{\partial N_i^{(eq)}}{\partial u_\alpha}} u_\alpha + \underbrace{\frac{1}{2} d(d-1) \left\{ (2d-1) b_1^2 c_{i\alpha} c_{i\beta} + 2a_2 \delta_{\alpha\beta} \right\}}_{\frac{\partial^2 N_i^{(eq)}}{\partial u_\alpha \partial u_\beta}} u_\alpha u_\beta$$

$\Rightarrow$

$$\rho = \sum_{i=0}^{5} N_i^{(eq)}$$

$$\rho \underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i^{(eq)}$$

Now:

$$\sum_{i=0}^{5} c_{i,\alpha} = 0$$

$$\sum_{i=0}^{5} c_{i\alpha} c_{i\beta} = 3\delta_{\alpha\beta}$$

$$\sum_{i=0}^{5} c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$

$c_{i,0}$ = [illegible] $\left(\frac{\pi}{3}\right)$ [illegible]

$c_{i,5}$ = [illegible] (0)

(2)

$$\Rightarrow \rho = \sum N_i^{(eq)} = \overset{N_i^{(eq)}(\rho,0)}{\rho} + \frac{1}{2} d(d-1)\left\{12 a_2 \delta_{\alpha\beta} + 3(2d-1) b_2^2 \delta_{\alpha\beta}\right\} u_\alpha u_\beta$$

$$\Rightarrow a_2 = \frac{(1-2d)^{5} b_2^2}{4} \Rightarrow a_2 = \frac{1-2d}{(d-1)^2}$$

(3)

$$\rho u_\beta = \sum \underline{c}_{i,\beta} N_i^{(eq)}$$

$$= d(d-1) b_2 \underbrace{\sum c_{i\alpha} c_{i\beta}}_{3\delta_{\alpha\beta}} u_\alpha = d(d-1) b_2 u_\beta \quad ; \quad \rho = 6d$$

$$\Rightarrow b_2 = \frac{2}{d-1}$$

$$\Rightarrow N_i^{(eq)} = d + 2d\, c_{i,\alpha} u_\alpha + \frac{d}{2(d-1)}\left\{2(1-2d)\delta_{\alpha\beta} + (2d-1)\, 4\, c_{i\alpha} c_{i\beta}\right\} u_\alpha u_\beta$$

$$= d + 2d(\underline{c}_i \cdot \underline{u}) + \underbrace{\frac{2d(2d-1)}{d-1}}_{\frac{\rho}{3}\left(\frac{2\rho-6}{\rho-6}\right) = G(\rho)} \underbrace{\left(c_{i\alpha} c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}\right)}_{\underline{\underline{Q}}_{\alpha\beta}} u_\alpha u_\beta$$

(2nd order tensor)

$$\boxed{N_i^{(eq)} = \rho\left\{\frac{1}{6} + \frac{\underline{c}_i \cdot \underline{u}}{3} + \frac{1}{3} G(\rho)\, Q_{\alpha\beta}\, u_\alpha u_\beta\right\}}$$

LGA equilibrium accurate up to 2nd order (Taylor expansion)

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LGA: $n_i(\underline{r}+\underline{c}_i, t+1) = n_i'(\underline{r},t)$

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t)$$

Conservation

$$\sum_{i=0}^{5} n_i' = \sum_{i=0}^{5} n_i \qquad N_i = \langle n_i \rangle \quad \left\{ \rho = \sum_{i=0}^{5} N_i \,,\; \rho \underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i \right\}$$

$$\sum_{i=0}^{5} \underline{c}_i n_i' = \sum_{i=0}^{5} \underline{c}_i n_i \qquad (1)\; \sum_{i=0}^{5} \langle n_i \rangle = \sum_{i=0}^{5} N_i(\underline{r},t) = \sum_{i=0}^{5} N_i(\underline{r}+\underline{c}_i, t+1)$$

$$(2) \qquad \sum \underline{c}_i N_i(\underline{r},t) = \sum \underline{c}_i N_i(\underline{r}+\underline{c}_i, t+1)$$

Multiscale expansion

Step 1: $N_i(\underline{r},t) = N_i^{(0)} + \varepsilon N_i^{(1)} + \varepsilon^2 N_i^{(2)} + \dots \qquad \varepsilon = O(N^{-1})$

$$N_i^{(eq)} = \frac{\rho}{6} + \frac{\rho}{3}(\underline{c}_i \cdot \underline{u}) + \frac{\rho}{3} G(\rho)\, Q_{i\alpha\beta}\, u_\alpha u_\beta$$

$$\boxed{G(\rho) = \frac{2\rho - 6}{\rho - 6} \;;\; Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}.}$$

$$\sum N_i^{(eq)} = \rho \qquad \Rightarrow \qquad \sum_{i=0}^{5} N_i^{(k)} = 0 \qquad k = 1, 2, 3, \dots$$

$$\sum \underline{c}_i N_i^{(eq)} = \rho \underline{u} \qquad\qquad \sum_{i=0}^{5} \underline{c}_i N_i^{(k)} = 0$$

Step 2:

Three relevant time scales

$t = t^{(0)}$ "noise"

$t^{(1)} = \varepsilon t \;;\; \varepsilon = O(N^{-1})$ "convection"

$t^{(2)} = \varepsilon^2 t \;;$ "diffusion"

multiscale modeling

$t^{(0)}$ = averaged out

assume $g(t^{(1)}(t), t^{(2)}(t))$ $\qquad ; \; \frac{\partial}{\partial t} = \partial_t = \frac{\partial}{\partial t^{(1)}}\frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}}\frac{\partial t^{(2)}}{\partial t}$

$$\frac{\partial}{\partial r_\alpha} \quad \partial r_\alpha = \varepsilon\, \partial r_\alpha^{(1)}$$

Step 3

Taylor expansion

$N_i(\underline{r}+\underline{c}_i, t+1)$, want to use (1) (2)

$$\Rightarrow N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \varepsilon \partial_{r_\alpha}^{(1)} N_i c_{i,\alpha} + \varepsilon \partial_t^{(1)} N_i + \varepsilon^2 \partial_t^{(2)} N_i + \text{higher order terms}$$

substitute with expansion: $N_i^{(0)} + \varepsilon N_i^{(1)} + \varepsilon^2 N_i^{(2)} + \dots$

Take moments in (1) and collect terms.

$$\varepsilon^1 : \partial_t^{(1)} \underbrace{\sum_{i=0}^{5} N_i}_{\rho} + \partial_{r_\alpha}^{(1)} \underbrace{\sum_{i=0}^{5} c_{i,\alpha} N_i}_{\rho u_\alpha} = 0$$

if $\partial t^{(1)}$ is [illegible] ; Now, this [illegible] is [illegible] the $\partial_t \rho + \partial_\alpha \rho u = 0$

End of Preview

Problems with LGA

- Noise problem – need to [illegible] time [illegible] average over the noise. (expensive) lots of averaging over time steps.
- inconsistency in momentum equation – partly [illegible] of $G(\rho)$ term
- Viscosity
- complexity of collision operator (2^6) – # bits, 6 for our case.

From ~~LBM~~ LGA to LBM

LGA $\quad n_i(\underline{r} + \underline{c}_i, t+1) = n_i(\underline{r}, t) + \Delta_i(\underline{r}, t)$

$$\Delta_i = \sum_{s,s' \in S} (s_i' - s_i) \underbrace{\xi_{s,s'}}_{\text{random bit}} \underbrace{\prod_{j=0}^{5} n_j^{s_j} (1 - n_j)^{1 - s_j}}_{\delta_{n,s}} \qquad (3)$$

Step 1 Averaging the LGA

$$\langle n_i(\underline{r} + \underline{c}_i, t+1) \rangle = \langle n_i(\underline{r}, t) \rangle + \langle \Delta_i(\underline{r}, t) \rangle$$

$$N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \langle \Delta_i(\underline{r}, t) \rangle$$

split $n_i = \underbrace{\langle n_i \rangle}_{N_i} + \hat{n}_i$ (fluctuation)

$\Rightarrow \langle \hat{n}_i \rangle = 0$

$\langle N_i \rangle = N_i$

Substitute into (3)

$$\langle \Delta_i \rangle = \left\langle \sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} (N_j + \hat{n}_j)^{s_j} (1 - N_j - \hat{n}_j)^{1 - s_j} \right\rangle$$

$\langle N_i \hat{n}_j \rangle = N_i \langle \hat{n}_j \rangle = N_i \cdot 0 = 0$

Now: get items like $\langle (N_i + \hat{n}_i)(N_j + \hat{n}_j) \rangle = N_i N_j + \cancel{\langle N_i \hat{n}_j \rangle}^{0} + \cancel{\langle N_j \hat{n}_i \rangle}^{0} + \underbrace{\langle \hat{n}_i \hat{n}_j \rangle}_{\text{higher order terms, chosen to neglect}}$

$$\Rightarrow N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \underbrace{\sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} N_j^{s_j} (1 - N_j)^{1 - s_j}}_{C_i(N_j)}$$

$C_i(N_j)$, $C_i(N_j^{(eq)}) = 0$; $N = (N_0 \quad N_5)$

Summary:

- (+) Noise removed.
- (−) now susceptible to round-off errors.
- (−) increased storage requirements. 6 bit boolean → 6 × 8 bit floating number
- (−) everything else, notably complexity (2^6) flops.

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Step 2 Linearity collision operator

Denote

$$N_i^{(eq,0)} = N_i^{(eq)}\Big|_{\underline{u}=0}$$

Linearize around $\boxed{N_i^{(eq,0)}}$

(4) $$C_i(N) = \cancel{C_i(N^{(eq)},0)}\ C_i(N^{(eq,0)}) + \frac{\partial C_i}{\partial N_j}\Big|_{\underline{u}=0}(N_j - N_j^{(eq)}) + \frac{1}{2}\frac{\partial^2 C_i}{\partial N_j \partial N_k}(N_j - N_j^{(eq,0)})(N_k - N_k^{(eq,0)})$$

+ higher-order term.

collision eq. → 0 with $N^{(eq)}$

(5) $$0 = C(N^{(eq)}) = C_i(N^{(eq,0)}) + \frac{\partial C_i}{\partial N_j}\Big|_{\underline{u}=0}(N_j^{(eq)} - N_j^{(eq,0)}) + \frac{1}{2}\frac{\partial^2 C_i}{\partial N_j \partial N_k}(N_j^{(eq)} \cdots) + \cdots$$

(4) − (5)

$$C_i \approx \frac{\partial C_i}{\partial N_j}(N_j - N_j^{(eq)}) + \text{higher order terms.}$$

└ neglecting

$$\frac{\partial C_i}{\partial N_j} = \begin{pmatrix} \frac{\partial C_i}{\partial N_i} & & \frac{\partial C_i}{\partial N_j} \\ & & \\ \frac{\partial C_i}{\partial N_i} & & \frac{\partial C_i}{\partial N_j} \end{pmatrix} \quad 6\times 6 \text{ mat.}$$

$$\Rightarrow N_i(\underline{r}+\underline{c}_i, t+1) = N_i(\underline{r}, t) + \left(\frac{\partial C_i}{\partial N_j}\right)(N_j - N_j^{(eq)})$$

Fermi-Dirac distribution (equilibrium)

Note: ① Complexity now b^2 (before 2^b)

② rest as before.

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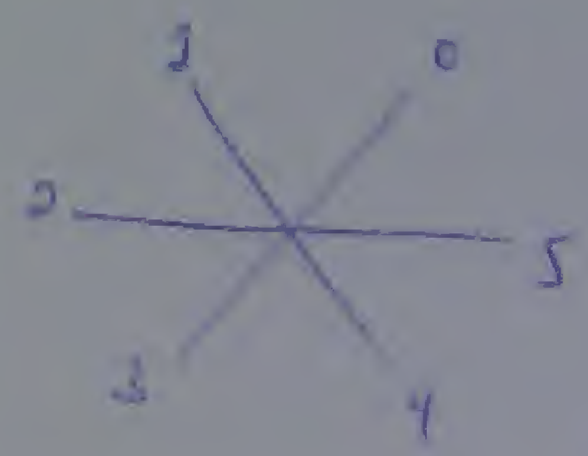
H - theorem for LGA



$n = (n_i)_{i=0,\dots,5}$
$= \cancel{(n_0\ n_1\ n_2\ n_3\ n_4\ n_5)}$
$= (n_5\ n_4\ n_3\ n_2\ n_1\ n_0)$

where $n_i \in \{0,1\}$

$N_i = \langle n_i \rangle = P(n_i = 1)$ — Probability of n_i occupied

$1 - N_i = P(n_i = 0)$ — n_i not occupied

Equilibrium

$$P(s \in S) = \prod_{j=0}^{5} N_j^{s_j} (1 - N_j)^{1-s_j} \quad (1) \qquad = N^{eq}$$

$S = \{0,1\}^6 = \{(s_5 \dots s_0) : s_i \in \{0,1\}\}$

this comes for independence of N_i's $\Rightarrow P(s = (111000)) = N_3 N_4 N_5 (1 - N_2)(1 - N_1)(1 - N_0)$

Let $P(s)$ be general probability of state $s \in S$, not necessarily (1)

$$\left(\sum_{s \in S} P(s) = 1 \right)$$

$$N_i = \sum_{s \in S} s_i P(s)$$

$$1 - N_i = \sum_{s \in S} (1 - s_i) P(s)$$

Now, Probability of $s' \in S$ after collision. (time t')

$$\underbrace{P'(s')}_{P(s;r,t')} = \sum_{s \in S} \langle \xi_{s,s'} \rangle \underbrace{P(s)}_{P(s;r,t)}$$

we had — sum of all possible allowed collision states

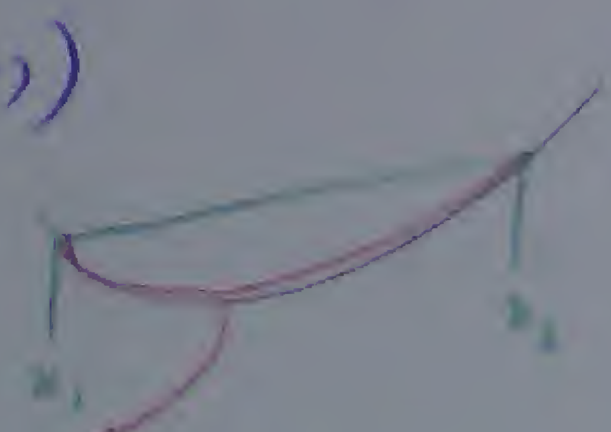
$$\sum_{s' \in S} \langle \xi_{s,s'} \rangle = 1 \quad (2)$$

$$\sum_{s \in S} \langle \xi_{s,s'} \rangle = 1 \quad (3)$$

Proposition:

for any convex function f,

$$\sum_{s'} f(P'(s')) \le \sum_{s} f(P(s))$$



proof:

Note f convex $\Rightarrow f(\xi x_1 + (1-\xi) x_2) \le \xi f(x_1) + (1-\xi) f(x_2)$; $\xi \in [0,1]$

Also holds for <u>convex combination</u> of n variables:

$$f\left(\sum_{j=1}^{n} \xi_j x_j\right) \leq \sum_{j=1}^{n} \xi_j f(x_j) \quad ; \quad \sum_{j=1}^{n} \xi_j = 1$$ ← convex combination sums to 1

$$\Rightarrow f\Big(\underbrace{\sum_{s \in S} \overbrace{\langle \xi_{s,s'} \rangle}^{=1,\ \text{from (1)}} P(s)}_{P(s')}\Big) \leq \sum_{s \in S} \langle \xi_{s,s'} \rangle f(P(s))$$

Sum over all $s' \in S$:

$$\sum_{s' \in S} f(P'(s')) \leq \sum_{s \in S} \underbrace{\sum_{s' \in S} \langle \xi_{s,s'} \rangle}_{=1} f(P(s))$$

$$= \sum_{s \in S} f(P(s)) \quad \blacksquare$$

$f = x \ln x$

$$\sum_{s'} P'(s') \ln P'(s') \leq \underbrace{\sum_{s} P(s) \ln P(s)}_{H(S,t)}$$

<u>Proposition</u>

$$\sum_{s \in S^*} P(s) \ln P(s) \geq \underbrace{\sum_{i=0}^{S} N_i \ln N_i + (1-N_i) \ln (1-N_i)}_{(*)}$$

with equality iff:

$$P(s) = \prod_{j=0}^{S} N_i^{s_i} (1-N_i)^{1-s_i}$$

<u>proof:</u>

$s_1 \ln(N_1) + s_2 \ln(N_2) = \ln(N_1^{s_1}) + \ln(N_2^{s_2})$

$= \ln\left(\prod_{i=1}^{2} N_i^{s_i}\right)$

$$N_i = \sum_{s \in S} s_i P(s)$$

$$1 - N_i = \sum_{s \in S} (1-s_i) P(s)$$

$$(*) = \sum_{i=0}^{S} \left(\sum_{s \in S} s_i P(s) \ln(N_i) + \sum_{s \in S} (1-s_i) P(s) \ln(1-N_i) \right)$$

$$= \sum_{s \in S} P(s) \left(\sum_{i=0}^{S} \left(s_i \ln(N_i) + (1-s_i) \ln(1-N_i) \right) \right)$$

$$= \sum_{s \in S} P(s) \left(\ln\left(\prod_{i=0}^{S} N_i^{s_i}\right) + \ln\left(\prod_{i=0}^{S} (1-N_i)^{1-s_i}\right) \right) = \sum_{s \in S} P(s) \ln\left(\prod_{i=0}^{S} N_i^{s_i} (1-N_i)^{1-s_i}\right)$$

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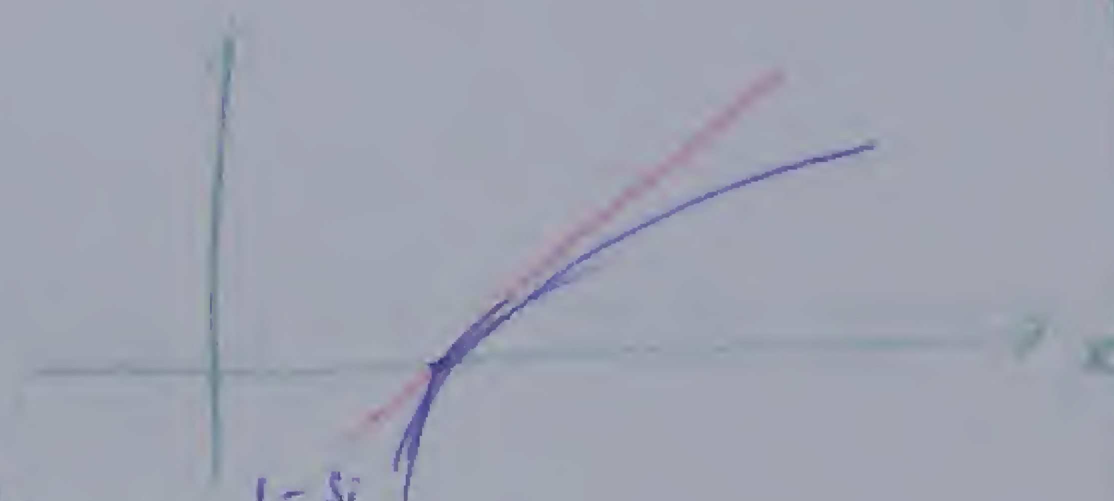
$$\overset{(4)}{\Rightarrow} \sum_{s \in S} P(s) \ln P(s) \geq \sum_{s \in S} P(s) \ln \left(\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i} \right)$$

$$\Rightarrow \sum_{s \in S} P(s) \ln \left(\frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} \right) \leq 0 \quad (*)$$

Note: get equality ~~at~~ iff

$$(5) \qquad P(s) = \prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}$$



otherwise, using $\ln x < x - 1 \quad (x \neq 1)$

$$\Rightarrow \ln \left(\frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} \right) < \frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} - 1$$

$$\sum_{s \in S} P(s) \ln \left(\ldots \right) < \sum_{s \in S} \cancel{P(s)} \left(\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i} - P(s) \right)$$

misleading! (5) doesn't hold! if compared to (*)

$$\text{r.h.s.} = \sum_{s \in S} \Big(\underbrace{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}_{P^{(M)}(s)} \Big) - 1$$

$= 0$

r.H.S. remains $= 0$ if (5) is used; otherwise, it is strictly less than 0.

$P^{(M)}(s)$, $s = (1\ 1\ 1\ 1\ 1\ 1)$

$\rightarrow N_0 N_1 N_2 N_3 N_4 N_5$

$$\sum_{s \in S} P^{(M)}(s) = N_0 N_1 N_2 N_3 N_4 N_5 + N_0 N_1 N_2 N_3 N_4 (1-N_5) + N_0 N_1 N_2 N_3 (1-N_4) N_5 + N_0 N_1 N_2 N_3 (1-N_4)(1-N_5)$$

$= 1$

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LGA: Equilibrium

$$N_i^{(eq)} = \frac{1}{1 + e^{a + \underline{b} \cdot \underline{c}_i}} \quad (\text{"Fermi - Dirac"})$$

work out $a, \underline{b}$ as functions of

$\rho \; (= \sum_i N_i)$

$\underline{u} \; (= \frac{1}{\rho} \sum_i \underline{c}_i N_i)$

$$N_i^{(eq)} \approx \rho \left(\frac{1}{6} + \frac{1}{3} c_{i\alpha} u_\alpha + G(\rho) \underbrace{Q_{i,\alpha\beta} u_\alpha u_\beta}_{(\underline{c}_i \cdot \underline{u})^2 - \frac{1}{2} u^2} \right) \text{ (small velocity approximation)}$$

$\underline{c}_i \cdot \underline{u}$

$G(\rho) = \frac{1}{3} \cdot \frac{6 - 2\rho}{6 - \rho}$ problematic

cause problems with NS

$Q_{i,\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{1}{2} \delta_{\alpha\beta}$

$\boxed{\text{LGA to LBM}}$

LGA is devised as attempt to bridge micro mechanics to macro scale dynamics (NS) also, there are terms that is not ... in the LBM will ... the errors with the problematic term.

Step 1 averaged LGA

$$N_i(\underline{r}_i + \underline{c}_i, t+1) = N_i(\underline{r}, t) + C_i(N), \quad N = (N_i)_{i=0,\dots,5}$$

$$C_i(N) = \sum_{s,s' \in \beta'} (s_i' - s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1 - N_j)^{1-s_j}$$

Note: $C_i(N^{(eq)}) = 0 \Rightarrow \sum_{i=0}^{5} C_i = 0, \quad \sum_{i=0}^{5} c_i C_i = 0$

Step 2. Linearize

$$N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \underbrace{\sum_{j=0}^{5} C_{ij}^{(0)} (N_j - N_j^{(eq)})}_{C_i(N)}$$

$\frac{\partial C_i}{\partial N_j} \Big|_{N^{(eq)}(\rho, u = 0)}$ (matrix)

Note: $C[N_i^{(eq)}] \Rightarrow \sum_{i=0}^{5} C_i = 0, \quad \sum_{i=0}^{5} c_i C_i = 0$

Step 3 "Model with enhanced collisions".

(a) In $N_i^{(eq)}$, we set $g(\rho) = \frac{1}{3} \cdot \boxed{\frac{6-2\rho}{6-\rho}} = 1$

$$\Rightarrow f_i^{(eq)} = \rho \left\{ \frac{1}{6} + \frac{1}{3} c_{i,\alpha} u_\alpha + \frac{1}{3} Q_{i,\alpha\beta} u_{\alpha\beta} \right\}$$

$$= \rho \left\{ \frac{1}{6} + \frac{1}{3} \underline{c}_i \cdot \underline{u} - \frac{u^2}{6} + \frac{1}{3} (\underline{c}_i \cdot \underline{u})^2 \right\}$$

Consider MB-distribution

$$f^{(MB)} = \frac{\rho}{(2\pi RT)} e^{-\frac{|c-u|^2}{2RT}} \quad \text{for 2D } \dots, \text{ in 3D } \frac{\rho}{(2\pi RT)^{3/2}}$$

$$= \boxed{\frac{\rho}{2\pi RT} e^{-\frac{c^2}{2RT}}}^{=A} \underbrace{e^{\frac{u\cdot c}{RT}} e^{-\frac{u^2}{2RT}}}_{(*)}$$

Note: $e^x = 1 + x + \frac{1}{2}x^2 + \dots$

$$\Rightarrow (*) = 1 + \frac{u\cdot c}{RT} - \frac{u^2}{2RT} + \frac{(c\cdot u)^2}{(RT)^2} + O(u^3)$$

$\boxed{A = \frac{\rho}{6} \quad RT = \frac{1}{2}}$, matches $f_i^{(eq)}$ ~~.....~~ $\neq$

4 (b) Replace $C_{ij}^{(0)}$ with

Matrix $A = (a_{ij})_{ij=1,\dots,b}$ satisfying conservation $\quad \sum C_i = 0, \quad \sum c_i C_i = 0 \quad ; C_i = \sum_j a_{ij}(f_j - f_j^{(eq)})$

Lattice-Boltzmann Method.

$$A_{ij} = -w\,\delta_{ij}$$

$$f(r + c_i, t+1) = f_i(r,t) + \overbrace{w\left(f^{(eq)}(r,t) - f_i(r,t)\right)}^{C_i \text{, collision operator}}$$

$$\left.\begin{aligned} \rho &= \sum f_i \overset{!}{=} \sum f_i^{(eq)} \\ \rho u &= \sum c_i f_i \overset{!}{=} \sum c_i f_i^{(eq)} \end{aligned}\right\} \Rightarrow \begin{cases} \sum C_i = \sum f_i - f_i^{(eq)} = 0 \\ \sum c_i C_i = \sum c_i(f_i - f_i^{(eq)}) = 0 \end{cases}$$

Remark:

Algorithm

init $f(r, t=0)\ \forall r$

do $n = 1, 2, 3, \dots$

$\quad \left.\begin{aligned} &\rho = \sum f_i \quad \rho u = \sum c_i f_i \\ &f_i^{(eq)} = f_i^{(eq)}(\rho, u) \\ &f_i' = w(f_i^{(eq)} - f_i) \end{aligned}\right\} \forall r \text{ locally}$

$\quad f(r + c_i, t+1) = f_i(r,t) + f_i'$ streaming

end do

$$f_i^{(eq)} = \rho w_i \left(1 + \frac{c_i \cdot u}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\frac{(c_i\cdot u)^2}{c_s^4}\right); \quad c_s^2 = RT$$

Computation of w_i

Review: Quadrature

$$I(f) = \int_a^b f \, dx \approx \sum_{i=1}^{n} \underbrace{\alpha_i}_{\text{weights}} \underbrace{f(x_i)}_{\text{nodes}} = I_n(f)$$

Def (degree of precision d.o.p)

We say $I_n(f)$ has d.o.p $m \in \mathbb{N}$ if $I(x^l) - I_n(x^l) = 0 \quad \forall l \leq m = 0, \dots, m.$

optimal quadrature rule:

gaussian $m = 2n - 1.$

Weighted Integrals

$$I^{(w)}(f) = \int_{a(-\infty)}^{b(\infty)} w(x) f(x) \, dx \approx \sum_{i=1}^{n} \alpha_i f(x_i) = I_n^{(w)}(f)$$

Still:

$$I^{(w)}(x^l) - I_n^{(w)}(x^l) = 0 \quad \text{for gaussian rule}, \; l = 0, \dots, 2n-1$$

Example

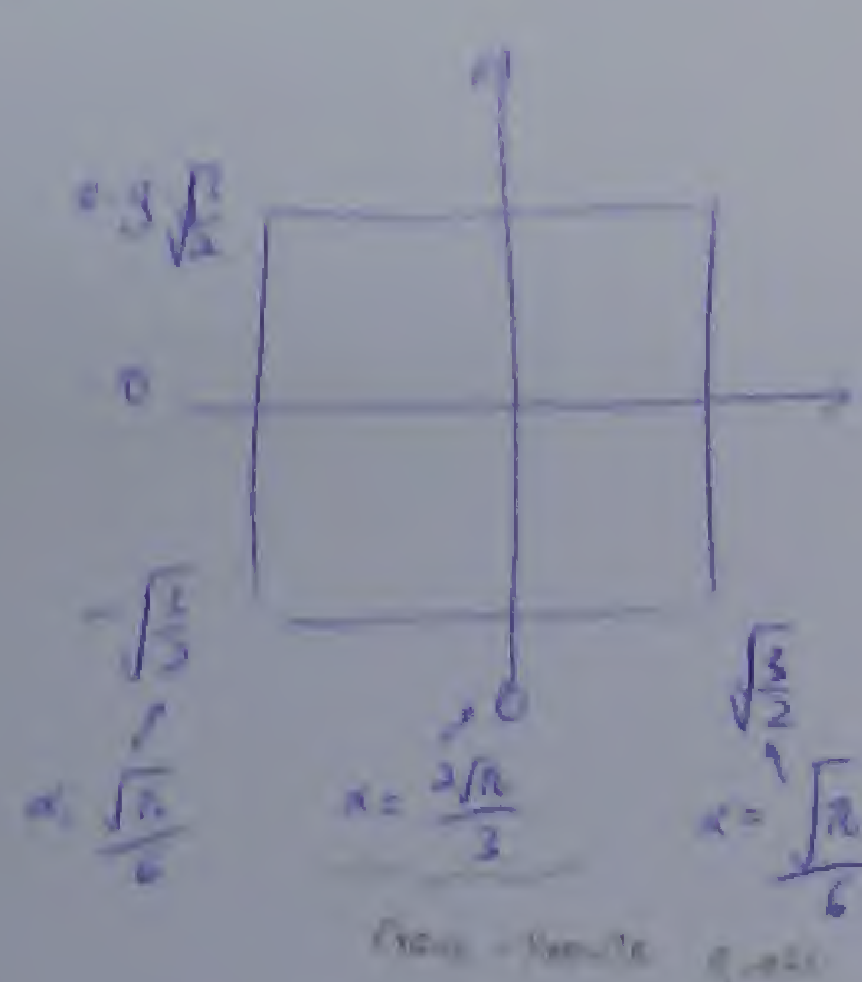
$w(x) = e^{-x^2}$ $\quad b = \infty$, $a = -\infty$

$\Rightarrow$ gauss - Hermite quadrature

Multivariate case

$$I^{(w)}(f) = \int_{\mathbb{R}^2} e^{-|x|^2} f(x) \, dx \, dy \; ; \; |x|^2 = x^2 + y^2$$

$$\approx \sum_{i,j=1}^{n} \underbrace{\alpha_i \beta_j}_{\text{weights, as in 1D}} f(x_i, y_j)$$



Recall:

$$f^{(eq)} = \underbrace{\frac{\rho}{2\pi RT} e^{-\frac{c^2}{2RT}}}_{A} \left(1 + \frac{c \cdot u}{RT} - \frac{u^2}{2RT} + \frac{1}{2} \cdot \frac{(c \cdot u)^2}{(RT)^2} \right)$$

$$\int_{\mathbb{R}^2} f^{(eq)} \, dc = \rho$$

$$\int_{\mathbb{R}^2} f^{(eq)} \, dc = \rho \underline{u}$$

Want:

$$\sum_{i=0}^{8} f_i^{(eq)} = \rho$$

$$\sum c_i f_i^{(eq)} = \rho \underline{u}$$

and possibly higher order moments (same as from M-B)

Consider:

$$I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^n c_2^m \, d\underline{c} \quad , \quad \tilde{f}^{(eq)} \text{ as in}$$

replace with Gauss-Hermite quadrature.

Multiscale Expansion

Consider ODE:

$$y(t) = a\cos(t) + b\sin(t)$$
$$y'(t) = a\cos(t) \cancel{+} - b\sin(t)$$
$$y'(t) = -a\sin(t) - b\cos(t)$$

(i) $y'' + y = 0 \Rightarrow y(t) = a\cos(t) + b\sin(t)$

$y(0) = 0 \qquad y(0) = 0 = a$

$y'(0) = 1 \qquad y'(0) = -b = 1$

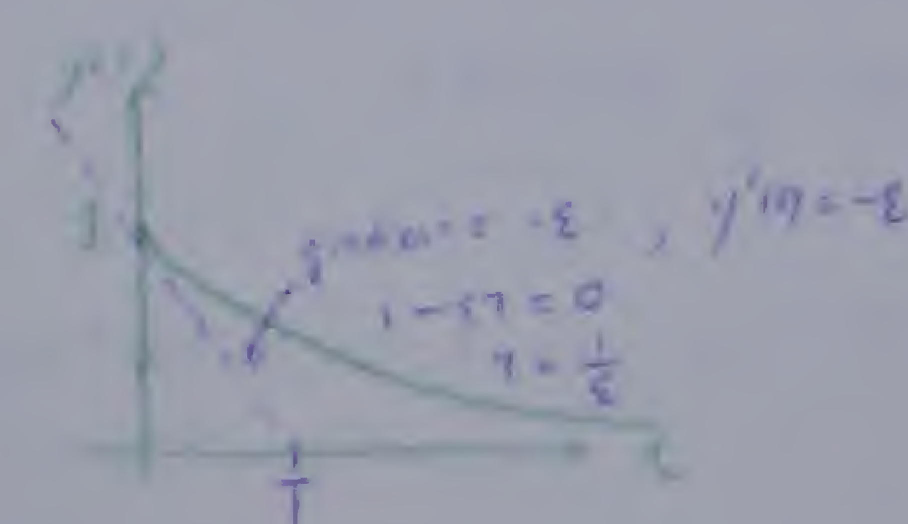
$\Rightarrow y(t) = b\sin(t) = -1\sin(t)$

Relevant time scale: $T = 2\pi = O(1)$

(ii) $y' + \varepsilon y = 0 \Rightarrow y(t) = a e^{-\varepsilon t}$

$y(0) = 1 \qquad y(0) = a = 1$

$y(t) = e^{-\varepsilon t}$



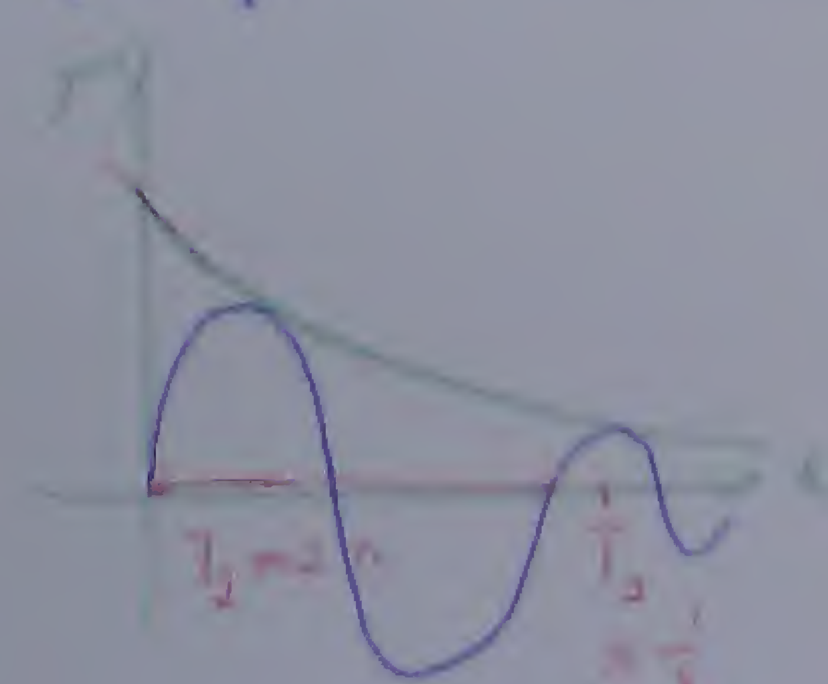
Relevant time scale: $T = \frac{1}{\varepsilon}$

$\boxed{\varepsilon \ll 1}$

(iii) $y'' + \varepsilon y' + y = 0 \quad \boxed{\varepsilon \ll 1} \Rightarrow y(t) = \frac{1}{\sqrt{1 - \frac{\varepsilon^2}{4}}} e^{-\frac{\varepsilon t}{2}} \sin\left(t \underbrace{\sqrt{1 - \frac{\varepsilon^2}{4}}}_{\approx 1}\right)$

$y(0) = 0$

$y'(0) = 1$



Perturbation Analysis problem (iii)

$$y(t) = \sum_{k=0}^{\infty} y_k(t)\, \varepsilon^k = y_0(t) + \varepsilon y_1(t) + O(\varepsilon^2)$$

Substitute into ODE eqn (iii): (neglect $O(\varepsilon^2)$ terms)

$$y_0'' + \varepsilon y_1'' + \varepsilon(y_0' + \cancel{\varepsilon y_1'}) + y_0 + \varepsilon y_1 = 0$$

$$y_0(0) + \varepsilon y_1(0) = 0$$

$$y_0'(0) + \varepsilon y_1'(0) = 1$$

Collect terms

$\varepsilon^0: \; y_0'' + y_0 = 0 \;\Rightarrow\; y(t) = \cancel{\sin(t)}\; a\sin(t) + b\cos(t)$

$y_0(0) = 0 \qquad \Rightarrow b = 0 = y(0)$

$y_0'(0) = 1 \qquad\;\; a = 1 = y'(0)$

$\Rightarrow y_0(t) = \sin(t)$

$\varepsilon^1: \; y_1'' + y_0' + y_1 = 0$

$\Rightarrow y_1'' + y_1 = -y_0' = -\cos(t)$

$y_1(0) = 0$

$y_1'(0) = 0$

$\Rightarrow y_1(t) = -\frac{1}{2} t \sin(t)$

$\Rightarrow y(t) = y_0(t) + \varepsilon y_1(t) = \sin(t) + \underbrace{\tfrac{1}{2}\varepsilon t \sin(t)}_{\geq 0}$

$|y(t)| \longrightarrow \infty \quad (t \longrightarrow \infty)$

here it will go to infinity instead of being [illegible] behaviour

$\boxed{\text{Multiscale (two-scale)}}$

Explicitly let y be a function of two time scales:

$$y(t) = \sum_{k=0}^{\infty} y_k(t_1(t), t_2(t))\, \varepsilon^k$$

$$t_1(t) = t$$

$$t_2(t) = \varepsilon t$$

$$y' = \frac{dy}{dt} = \frac{\partial y}{\partial t_1}\overbrace{\frac{\partial t_1}{\partial t}}^{=1} + \frac{\partial y}{\partial t_2}\overbrace{\frac{\partial t_2}{\partial t}}^{=\varepsilon}$$

$$= \frac{\partial y}{\partial t_1} + \frac{\partial y}{\partial t_2}\varepsilon$$

Substitute into ODE:

$$\partial_t(\partial_{t_1} y + \partial_{t_2} y\, \varepsilon) + \varepsilon(\partial_{t_1} y + \varepsilon \partial_{t_2} y) + y = 0$$

$$\partial_{t_1}^2 y + 2\varepsilon \partial_{t_1}\partial_{t_2} y + \cancelto{0}{\varepsilon^2 \partial_{t_2}^2 y} + \varepsilon \partial_{t_1} y + \cancelto{0}{\varepsilon^2 \partial_{t_2} y} + y = 0$$

$$\partial_{t_1}^2(y_0 + \varepsilon y_1) + 2\varepsilon \partial_{t_1}\partial_{t_2}(y_0 + \cancelto{0}{\varepsilon y_1}) + \varepsilon \partial_{t_1}(y_0 + \cancelto{0}{\varepsilon y_1}) + y_0 + \varepsilon y_1 \approx 0$$

$$y_0 + \varepsilon y_1 \big|_{t=0} = 0$$

$$\underbrace{\partial_{t_1}(y_0 + \varepsilon y_1) + \varepsilon \partial_{t_2}(y_0 + \varepsilon y_1)}_{\partial_t y} \Big|_{t=0} = 1$$

$\underline{\varepsilon^0}$: $\partial_{t_1}^2 y_0 + y_0 = 0 \Rightarrow y_0(t) = a_0(t_2)\sin(t_1) + b_0(t_2)\cos(t_1)$

$y_0(0) = 0$

$\partial_{t_1} y_0(0) = 1$

$y_0(0) = b_0(0) = 0 \quad (1)$

$\partial_{t_1} y_0(0) = a_0(0) = 1 \quad (2)$

$\underline{\varepsilon^1}$:

$\cancel{\partial_{t_1}^2 y_1 + 2\partial_{t_2} y_0}$

$\partial_{t_1}^2 y_1 + 2\partial_{t_1}\partial_{t_2} y_0 + \partial_{t_1} y_0 + y_1 = 0$

$\Rightarrow \partial_{t_1}^2 y_1 + y_1 = -2\partial_{t_1}\partial_{t_2} y_0 - \partial_{t_1} y_0$

$[\partial_{t_1} y_0 = a_0(t_2)\cos(t_1) - b_0(t_2)\sin(t_1)]$

$= -2\left(a_0'(t_2)\cos(t_1) + b_0'(t_2)\sin(t_1)\right) \underbrace{- a_0(t_2)\cos(t_1) + b_0(t_2)\sin(t_1)}_{\partial_{t_1} y_0(t)}$

$\Rightarrow \partial_{t_1}^2 y_1 + y_1 = -\underbrace{(2a_0' + a_0)}_{\stackrel{!}{=}0}\cos(t_1) + \underbrace{(2b_0' + b_0)}_{\stackrel{!}{=}0}\sin(t_1)$

[illegible]

<u>Kill growth terms</u>

$2a_0' + a_0 = 0 \Rightarrow a_0(t_2) = C e^{-\frac{t_2}{2}}$

$(2) \Rightarrow a_0(0) = 1 \Rightarrow C = 1$

$\left.\begin{array}{r} 2b_0' + b_0 = 0 \\ b_0(0) = 0 \end{array}\right\} b_0 \equiv 0$

$\Rightarrow y_0(t) = e^{-\frac{t_2}{2}} \sin(t)$

$= e^{-\frac{\varepsilon t}{2}} \sin(t)$

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Previously:

Linearized (averaged) LGA

$\left.\frac{\partial C_i(N)}{\partial N_j}\right|_{N=0}$ → collision operator of averaged LGA

$$N_i(\underline{r}+\underline{c}_i, t+1) = N_i(\underline{r}, t) + C_{ij}^{(lin)}\left(N_j(\underline{r}, t) - N_j^{(eq)}\right)$$

In LBM $C(N)$ and $N_j^{(eq)}$ is chosen for consistency with conservation laws, thereby [illegible] no relation with LGA [illegible].

Conservation:

$C_i^{(lin)}(N^{(eq)}) = 0$

$\sum_i C_i^{(lin)} = 0$

$\sum_i c_i C_i^{(lin)} = 0$

$$f_i(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega\left(\underbrace{f_i^{(eq)}(\underline{r}, t) - f_i(\underline{r}, t)}_{C_i}\right)$$

$$f_i^{(eq)} = \rho w_i\left(1 + \frac{\underline{c}_i \cdot \underline{u}}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\cdot\frac{(\underline{c}_i\cdot\underline{u})^2}{(RT)^2}\right) \; ; \; c_s^2 = RT$$

w_i: [illegible] weights, constants.

Note:

$$\rho(\underline{r}, t) = \sum_i f_i(\underline{r}, t)$$

$$\rho\underline{u} = \sum_i \underline{c}_i f_i$$

Determine w_i s.th.

$$\sum_i f_i^{(eq)} c_{i,1}^m c_{i,2}^n = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2 \; ; \; \underline{c}_i = (c_{i,1} \;\; c_{i,2})^T$$

to some degree m, n.

$$\tilde{f}^{(eq)} = \frac{\rho}{2\pi RT} e^{-\frac{c^2}{2RT}}\left\{1 + \frac{\underline{c}\cdot\underline{u}}{RT} - \frac{u^2}{2RT} + \frac{1}{2}\frac{(\underline{c}\cdot\underline{u})^2}{(RT)^2}\right\} \; ;$$

Known: $\int_{\mathbb{R}^2} \tilde{f}^{(eq)} d\underline{c} = \rho$

$\int_{\mathbb{R}^2} \tilde{f}^{(eq)} \underline{c} \, d\underline{c} = \rho\underline{u}$

In particular, then we have

$$\sum_i f_i^{(eq)} = \rho = \sum_i f_i \Rightarrow \sum_i C_i = 0$$

$$\sum_i \underline{c}_i f_i^{(eq)} = \rho\underline{u} = \sum_i f_i \underline{c}_i \Rightarrow \sum_i \underline{c}_i C_i = 0$$

Recall: Gauss-Hermite Quadrature:

$$\int_{\mathbb{R}} e^{-x^2} g(x) = \sum_{i=1}^{n} w_i g(x_i) + R_n$$

Set $\underline{c} = \sqrt{2RT}\,\underline{\xi}$

Then $I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2$

$$= \frac{\rho}{\pi}(2RT)^{\frac{m+n}{2}} \int_{\mathbb{R}^2} \xi_1^m \xi_2^n e^{-\xi^2}\left(1 + \frac{\sqrt{2}\,\underline{\xi}\cdot\underline{u}}{\sqrt{RT}} - \frac{u^2}{2RT} + \frac{(\underline{\xi}\cdot\underline{u})^2}{RT}\right) d\xi_1 d\xi_2$$

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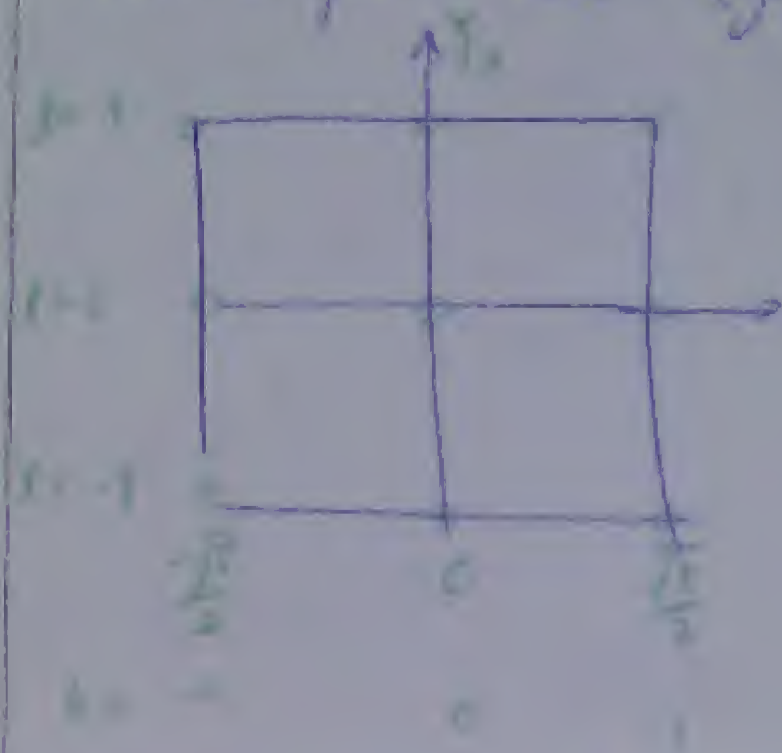
Use 3 point Rule : (Gauss – Hermite)

LBM $f^{(eq)}_i = \rho w_i \left(1 + \frac{c_i \cdot u}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\frac{(c_i \cdot u)^2}{(c_s^2)^2}\right)$



$w_0 = \frac{2\sqrt{\pi}}{3}$

$w_1 = w_{-1} = \frac{\sqrt{\pi}}{6}$

$$\Rightarrow I \simeq \rho (2RT)^{\frac{m+n}{2}} \sum_{k,l=-1}^{1} \frac{w_k w_l}{\pi} \xi_{1,k}^m \xi_{2,l}^n \left\{1 + \frac{\sqrt{2}(\xi_{1,k} u_1 + \xi_{2,l} u_2)}{\sqrt{RT}} - \frac{u^2}{2RT} + \frac{(\xi_{1,k} u_1 + \xi_{2,l} u_2)^2}{RT}\right\}$$

Note : $\xi_{1,k} u_1 + \xi_{2,k} u_2$

$= \sqrt{\frac{3}{2}} (k u_1 + l u_2)$

$= \frac{\sqrt{3}}{\sqrt{2}} (\tilde{c}_{k,l} \cdot \underline{u})$; $\tilde{c}_{k,l} = (k,l)^T$

and :

$$\frac{w_k w_l}{\pi} = \begin{cases} 4/9 & k = l = 0 \\ 1/9 & k = 0 \;\; l \neq 0 \\ & l = 0 \;\; k \neq 0 \\ 1/36 & |k| = |l| = 1 \end{cases}$$

Set $\tilde{u} = \frac{u}{\sqrt{2RT}}$

$$f_i^{(eq)} = \begin{cases} 4/9\, \rho \{1 - \frac{3}{2} u^2\} & , i = 0 \\ 1/9\, \rho \{1 + 3 \tilde{c}_i \cdot \tilde{\underline{u}} + \frac{9}{2} (\tilde{c}_i \cdot \tilde{\underline{u}})^2 - \frac{3}{2} \tilde{u}^2\} & , i = 1, 2, 3, 4 \\ 1/36\, \rho \{ \cdots \} & , i = 5, 6, 7, 8 \end{cases}$$

$\rho = \sum f_i$

$\rho u = \sum c_i f_i$

Claim! the procedure satisfies NS equ...

Multiscale expansion

Recall : LBM D2Q9 , 2D , 9 point Quadrature

(1) $f_i(\underline{r} + c_i, t+1) = f_i(\underline{r}, t) + \omega (f_i(\underline{r}, t) - f_i^{(eq)}(\underline{r}, t))$

(2) $\sum_{i=0}^{8} f_i^{(eq)} = \sum_{i=0}^{8} f_i = \rho$

(3) $\sum_{i=0}^{8} c_i f_i^{(eq)} = \sum_{i=0}^{8} c_i f_i = \rho \underline{u}$

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Relevant Scales (spatial and temporal)

Let $\varepsilon = \frac{1}{N}$

① Lattice "Knudsen" number $= \frac{\Delta x}{L} = O(\varepsilon) = O\left(\frac{1}{N}\right)$

② ⓘ convective scale $O(N)$
ⓘ diffusive scale $O(N^2)$

Scaled coordinates:

$r_\alpha^{(1)} = \varepsilon \underline{r}_\alpha$

$t^{(1)} = \varepsilon t \qquad t = N = \frac{1}{\varepsilon} \Rightarrow t^{(1)} = 1$

$t^{(2)} = \varepsilon^2 t \qquad t = N^2 = \frac{1}{\varepsilon^2} \Rightarrow t^{(2)} = 1$

$$\left.\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial}{\partial t^{(1)}}\frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}}\frac{\partial t^{(2)}}{\partial t} \\ &= \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)} \\ \frac{\partial}{\partial r_\alpha} &= \varepsilon \partial_\alpha^{(1)} \end{aligned}\right\} \quad (**)$$

Need to expand:

$$f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)} = \sum_{k=0}^{\infty} \varepsilon^k f^{(k)}\left(r^{(1)}(r), t^{(1)}(t), t^{(2)}(t)\right)$$

$$\left. f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \dots \right\} \quad (***)$$

$$f_i(\underline{r} + \underline{c}_i \Delta t, t + \Delta t) = f_i(\underline{r}, t) + \partial_{r_\alpha} f_i c_{i\alpha} \Delta t + \partial_t f_i \Delta t + \frac{1}{2}(\Delta t)^2 \{\partial_t \partial_t f_i + 2 c_{i\alpha} \partial_{r_\alpha} \partial_t f_i + c_{i\alpha} c_{i\beta} \partial_\alpha \partial_\beta f_i\} \quad (*)$$

substitute $(*)$ into (1)

$$\Rightarrow \partial_{r_\alpha} f_i c_{i\alpha} \Delta t + \partial_t f_i \Delta t + \frac{(\Delta t)^2}{2}\{\quad\} - \omega(f_i^{(eq)} - f_i) = 0$$

substitute $(**)$ $(***)$ into ↑

$$\Rightarrow E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} + \dots = 0$$

$E_i^{(m)}$ contain only such terms $\partial_t^{(k)} f_i^{(l)}$ with $k + l = m$

$E_i^{(0)} = 0$ if $f_i^{(0)} = f_i^{(eq)}$

$E_i^{(1)} = \partial_\alpha^{(1)} f_i^{(0)} \Delta t + \partial_t^{(1)} f_i^{(0)} \Delta t + \omega f_i^{(1)}$

$E_i^{(2)} = \partial_\alpha^{(1)} f_i^{(1)} \Delta t + \Delta t \partial_t^{(2)} f^{(0)} + \Delta t \partial_t^{(1)} f^{(1)} + \frac{1}{2}(\Delta t)^2 (\partial_t^{(1)} \partial_t^{(1)} f_i^{(0)} + 2 c_{i\alpha} \partial_\alpha^{(1)} \partial_t^{(1)} f_i^{(0)} + c_{i\alpha} c_{i\beta} \partial_\alpha^{(1)} \partial_\beta^{(1)} f^{(0)}) + \omega f^{(2)}$

Moments

(A) $\sum_i E_i^{(1)}$

(B) $\sum_i \underline{c}_i E_i^{(1)}$

(C) $\sum_i E_i^{(2)}$

(D) $\sum_i \underline{c}_i E_i^{(2)}$

claim: ← will be apparent!

(A) + ε(B) $= 0$

(C) + ε(D) $= 0$

consistent with Navier-stokes.

30th Jan 2017

Review

Multiscale Expansion.

(LBM)

(1) $f_i(\underline{r}+\underline{c}_i\Delta t,\ t+\Delta t) = f_i(\underline{r},t) + \omega\left(f_i^{eq}(\underline{r},t) - f_i(\underline{r},t)\right)$, $i = 0, \dots, 9$

$$f_i^{(eq)} = \rho w_i \left(1 + 3(\underline{c}_i\cdot\underline{u}) - \tfrac{3}{2}u^2 + \tfrac{9}{2}(\underline{c}_i\cdot\underline{u})^2\right)$$

(2) $\sum_{i=0}^{8} f_i(\underline{r},t) = \sum_{i=0}^{8} f_i^{(eq)}(\underline{r},t) = \rho$

(3) $\sum_{i=0}^{8} \underline{c}_i f_i(\underline{r},t) = \sum_{i=0}^{8} \underline{c}_i f_i^{(eq)}(\underline{r},t) = \rho\underline{u}$

Relevant (spatial & temporal) scales

Let $\varepsilon = \frac{1}{N}$

(*) "Lattice Knudsen" number $\frac{\Delta x}{L} = O(N^{-1}) = O(\varepsilon)$ ← char length scale

(*) (i) Convective timescale $O(N)$

(ii) diffusive timescale $O(N^2)$

Introduce Scaled Coordinates

$\underline{r}^{(1)} = \varepsilon\underline{r}$ $r = N \Rightarrow r^{(1)} = 1$

$t^{(1)} = \varepsilon t$ $t = N \Rightarrow t^{(1)} = 1$

$t^{(2)} = \varepsilon^2 t$ $t = N^2 \Rightarrow t^{(2)} = 1$

we will set $f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)}$

$$f_i^{(k)} = f_i^{(k)}\left(r^{(1)},\ t^{(1)}(t),\ t^{(2)}(t)\right)$$

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$$\frac{\partial}{\partial t} = \frac{\partial t^{(1)}}{\partial t}\frac{\partial}{\partial t^{(1)}} + \frac{\partial t^{(2)}}{\partial t}\frac{\partial}{\partial t^{(2)}}$$

$$\Rightarrow \partial_t = \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)}$$

$$\frac{\partial}{\partial r} = \varepsilon \frac{\partial}{\partial r^{(1)}} \quad (4)$$

$$\Rightarrow \partial_{r_\alpha} = \varepsilon \partial_{r_\alpha}^{(1)} \quad , \alpha = 1, 2$$

here $f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \ldots$ (5)

Note: $\sum_i f_i^{(k)} = 0$ $\quad k \geq 1 \quad (f^{(0)} = f^{(eq)})$

$\sum_i c_i f_i^{(k)} = 0$

$$f_i(r + c_i t, t + \Delta t) = f_i(r,t) + c_{i,\alpha}\Delta t\, \partial_\alpha f_i + \partial_t f_i \Delta t + \frac{\Delta t^2}{2}\left\{\partial_t \partial_t f_i + 2 c_{i\alpha}\partial_\alpha \partial_t f_i + c_{i\alpha} c_{i\beta} \partial_\alpha \partial_\beta f_i\right\} + \mathcal{O}(\Delta t^3) \quad (6)$$

symmetric

will do later

Substitute (6) into (1)

$$c_{i,\alpha}\Delta t\, \partial_\alpha f_i + \Delta t\, \partial_t f_i + \frac{\Delta t^2}{2}\{\cdots\} - \omega(f^{(eq)} - f_i) \approx 0 \quad (7)$$

Substitute (4) (5) into (7)

$$(7) \Rightarrow E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} + \ldots$$

where each $E^{(k)}$ contains terms like

$$\partial_t^{(l)} f^{(m)} \quad \text{s.t. } l + m = k$$

$$E_i^{(0)} = f^{(0)} - f^{(eq)}$$

Since $f^{(0)}, f^{(1)}, f^{(2)}$, ... are lin. indep. $E_i^{(k)} = 0$.

$$E_i^{(1)} = c_{i,\alpha}\Delta t\, \partial_\alpha^{(1)} f^{(0)} + \Delta t\, \partial_t^{(1)} f_i^{(0)} + \omega f^{(1)}$$

$$E_i^{(2)} = \Delta t\, \partial_t^{(1)} f_i^{(1)} + \Delta t\, \partial_t^{(2)} f_i^{(0)} + c_{i,\alpha}\Delta t\, \partial_\alpha^{(1)} f^{(1)} + \frac{\Delta t^2}{2}\left\{\partial_t^{(1)}\partial_t^{(1)} f^{(0)} + 2c_{i\alpha}\partial_\alpha^{(1)}\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}c_{i\beta}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)}\right\} - \omega f^{(2)}$$

<u>Moments:</u>

(A) $\sum_{i=0}^{8} E_i^{(1)}$ $\qquad$ (C) $\sum E_i^{(2)}$

(B) $\sum c_i E_i^{(1)}$ $\qquad$ (D) $\sum c_i E_i^{(2)}$

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(2)

Claim:

$$\sum E_i^{(1)} + \varepsilon E_i^{(2)} = 0$$ "gives" N-S.

$$\sum c_i \left(E_i^{(1)} + \varepsilon E_i^{(2)}\right) = 0$$

(A) $$\frac{1}{\Delta t}\sum_i E_i^{(1)} = \sum_i \partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} f_i^{(1)}$$

$$= \partial_t^{(1)}\underbrace{\left(\sum_i f_i^{(0)}\right)}_{\rho} + \partial_\alpha^{(1)}\underbrace{\left(\sum_i c_{i\alpha} f_i^{(0)}\right)}_{\rho u_\alpha}$$

$$= \partial_t^{(1)}\rho + \partial_\alpha^{(1)}(\rho u_\alpha)$$

(B) $$\frac{1}{\Delta t}\sum c_i E_i^{(1)} = \sum c_{i\alpha}\partial_t^{(1)} f_i^{(0)} + \sum_i c_{i\alpha} c_{i\beta}\partial_\beta^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t}\sum_i f_i^{(1)} c_{i\alpha}$$

$$= \partial_t^{(1)}\underbrace{\left(\sum_i c_{i\alpha} f_i^{(0)}\right)}_{\rho u_\alpha} + \partial_\beta^{(1)}\underbrace{\left(\sum_i c_{i\alpha} c_{i\beta} f_i^{(0)}\right)}_{P_{\alpha\beta}^{(0)}}$$

(C) $$\frac{1}{\Delta t}\sum_i E_i^{(2)} = \partial_t^{(2)}\rho + \frac{\Delta t}{2}\left\{\partial_t^{(1)}\partial_t^{(1)}\rho + 2\partial_\alpha^{(1)}\partial_t^{(1)}\rho u_\alpha + \partial_\alpha^{(1)}\partial_\beta^{(1)} P_{\alpha\beta}^{(0)}\right\} - \frac{\omega}{\Delta t} f^{(2)}$$

$$= \partial_t^{(2)}\rho + \frac{\Delta t}{2}\left[\partial_t^{(1)}\underbrace{\left(\partial_t^{(1)}\rho + \partial_\alpha^{(1)}\rho u_\alpha\right)}_{E(A)=0} + \partial_t^{(1)}\partial_\alpha^{(1)}\rho u_\alpha + \partial_\alpha^{(1)}\partial_\beta^{(1)} P_{\alpha\beta}^{(0)}\right]$$

$$= \partial_t^{(2)}\rho + \frac{\Delta t}{2}\partial_\alpha^{(1)}\underbrace{\left\{\partial_t^{(1)}\rho u_\alpha + \partial_\beta^{(1)} P_{\alpha\beta}\right\}}_{E(B)=0}$$

$$\rightarrow \frac{\varepsilon}{\Delta t}\sum E_i^{(2)} + \frac{\varepsilon^2}{\Delta t}\sum E_i^{(2)} = \varepsilon\partial_t^{(1)}\rho + \varepsilon^2\partial_t^{(2)}\rho + \varepsilon\partial_\alpha^{(1)}(\rho u_\alpha)$$

$$= \partial_t\rho + \partial_\alpha(\rho u_\alpha) = 0$$

Need to finish moment (B)

(B) $$= \frac{1}{\Delta t}\sum c_{i\alpha} E_i^{(1)} = \partial_t^{(1)}\rho u_\alpha + \partial_\beta^{(1)}\underbrace{\left(c_{i\alpha} c_{i\beta} f^{(0)}\right)}_{P_{\alpha\beta}^{(0)}}$$

$$P_{\alpha\beta}^{(0)} = \sum c_{i\alpha} c_{i\beta}\rho w_i\left\{1 + 3(c_i\cdot u) - \frac{3}{2}u^2 + \frac{9}{2}(c_i\cdot u)^2\right\}$$

$$= P_{\alpha\beta}^{(0,1)} + P_{\alpha\beta}^{(0,2)} + P_{\alpha\beta}^{(0,3)} + P_{\alpha\beta}^{(0,4)}$$

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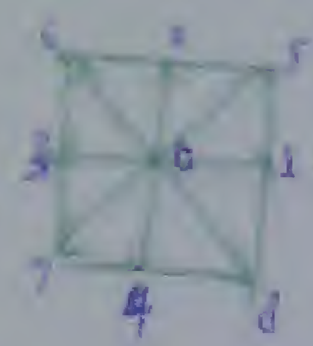
LBM . . 23rd Dec 2016

$\frac{\partial}{\partial t}$ $P_{\alpha\beta}^{(0,1)} = \rho \sum_i w_i \, c_{i,\alpha} \, c_{i,\beta} = \rho \frac{1}{3} \delta_{\alpha\beta}$



$\Rightarrow \partial_t$ $\quad W_0 = \frac{4}{9} \quad w_i^* = \frac{1}{9} \quad i = 1, \dots, 4$

$\frac{\partial}{\partial r}$ $\quad w_i^* = \frac{1}{36} \quad i = 5, \dots, 8$

$\Rightarrow \partial_{r_1}$ e.g. $\alpha = \beta = 1$

here $\sum w_i \, c_{i,\alpha=1}^2 = 2 \cdot \frac{1}{9} + \frac{4}{36} = \frac{1}{3}$

No Recall: $c_{i,\alpha}^* = C_0^*$ $\qquad (C_s^*)^2 = RT^*$

dimensional

$\left(\frac{C_0^*}{C_s^*}\right)^2 = 3$

$\Rightarrow \frac{1}{3} = \left(\frac{C_s^*}{C_0^*}\right)^2 = \frac{RT^*}{C_0^2}$, Also $\rho = \frac{\rho^*}{\rho_{ref}}$

$\Rightarrow P_{\alpha\beta}^{(0,1)} = \frac{\rho^*}{\rho_{ref}} \cdot \frac{RT^*}{(C_0^*)^2} \delta_{\alpha\beta} = \frac{P^*}{\rho_{ref}} \frac{\delta_{\alpha\beta}}{(C_0^*)^2} = p \, \delta_{\alpha\beta}$

Also:

$P_{\alpha\beta}^{(0,2)} = 3 \rho u_\gamma \sum w_i c_{i,\alpha} c_{i,\beta} c_{i,\gamma} = 0$

$P_{\alpha\beta}^{(0,3)} = -\frac{3}{2} (u_1^2 + u_2^2) \rho \sum w_i \, c_{i,\alpha} c_{i,\beta} \, \delta_{\alpha\beta} = -\frac{1}{2} (u_1^2 + u_2^2) \rho \, \delta_{\alpha\beta}$

$P_{\alpha\beta}^{(0,4)} = \frac{9}{2} \rho \sum_i w_i \, c_{i,\alpha} c_{i,\beta} (\underline{c}_i \cdot \underline{u})^2 \Rightarrow P_{\alpha\beta}^{(0,4)} = \begin{cases} \frac{3}{2}\rho u_1^2 + \frac{1}{2}\rho u_2^2 & \alpha = \beta = 1 \\ \rho u_\alpha u_\beta & \alpha \neq \beta \\ \frac{1}{2}\rho u_1^2 + \frac{3}{2}\rho u_2^2 & \alpha = \beta = 2 \end{cases}$

$P_{11}^{(0)} = p + \frac{1}{2} (u_1^2 + u_2^2) \rho + \frac{3}{2} \rho u_1^2 + \frac{1}{2} \rho u_2^2$

$= p + \rho u_1^2$

Similarly, $P_{\alpha\beta}^{(0)} = \rho u_\alpha u_\beta \quad (\alpha \neq \beta)$

$P_{22}^{(0)} = p + \rho u_2^2$

$P_{\alpha\beta}^{(0)} = p \, \delta_{\alpha\beta} + \rho u_\alpha u_\beta$

$\frac{1}{\Delta t} \sum c_{i,\alpha} E_i^{(1)} = \partial_t^{(1)} (\rho u_\alpha) + \partial_\beta^{(1)} P_{\alpha\beta}^{(0)} = \partial_t^{(1)} (\rho u_\alpha) + \partial_\alpha^{(1)} p + \partial_\beta^{(1)} (\rho u_\alpha u_\beta)$

LBM 1-12-11

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A $\sum_i E^{(1)}$ $\Rightarrow \varepsilon A + \varepsilon^2 B = 0$ $= \partial_t(\rho h_\alpha) + \partial_\beta(\rho h_\beta)$

B $\sum_i c_{i\alpha} E_i^{(1)}$ $\varepsilon C + \varepsilon^2 D = 0$ okay!

C $\sum_i E_i^{(2)}$ $\partial_t^{(1)}(\rho h_\alpha) + \partial_\beta^{(1)}(\rho h_\alpha h_\beta) + \partial_\alpha P$

D $\sum_i c_{i\alpha} E_i^{(2)}$

$$\frac{1}{\Delta t} E_i^{(2)} = \partial_t^{(1)} f_i^{(1)} + \partial_t^{(2)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(1)} + \frac{1}{2}\Delta t\left(\partial_t^{(1)}\partial_t^{(1)} f_i^{(0)} + 2c_{i\alpha}\partial_t^{(1)}\partial_\alpha^{(1)} f_i^{(0)} + c_{i\beta}c_{i\alpha}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)}\right) + \frac{\omega}{\Delta t} f_i^{(2)}$$

$$\Rightarrow \frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(2)} = \partial_t^{(1)}(\rho h_\alpha) + \partial_\beta^{(1)}\sum_i c_{i\alpha}c_{i\beta} f_i^{(1)} + \frac{1}{2}\Delta t\Big(\partial_t^{(1)}\partial_t^{(1)}(\rho h_\alpha) + 2\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \underbrace{\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)}}_{(**)}\Big)$$

$\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)}$

$$\frac{1}{\Delta t} E^{(1)} = \partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} f_i^{(1)} \quad (*)$$

formally let $\varepsilon \to 0$ $\Rightarrow \varepsilon A + \varepsilon^2 B = 0$

$$f_i^{(1)} = -\frac{\Delta t}{\omega}\left\{\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)}\right\}$$

$$\Rightarrow \frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(2)} = \partial_t^{(2)}(\rho h_\alpha) - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_t^{(1)}\underbrace{\sum_i c_{i\alpha}c_{i\beta} f_i^{(0)}}_{P_{\alpha\beta}} - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)} + \frac{1}{2}\Delta t\{(**)\}$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(1 - \frac{1}{\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\frac{1}{2} - \frac{1}{\omega}\right)\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)}$$

$$+ \frac{1}{2}\Delta t\,\underbrace{\partial_t^{(1)}\partial_t^{(1)}(\rho u_\alpha)}_{\text{disappears } (\varepsilon \to 0)}$$

Recall momentum:

$$\partial_t(\rho u_\alpha) + \underbrace{\partial_\beta(\rho u_\alpha u_\beta) + \partial_\alpha P}_{\partial_\beta P_{\alpha\beta}} = \mathcal{O}(\varepsilon)$$

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$$H^{(q)} = \sum_{x \in} \left[\underbrace{\sum_i h_i(f_i(x,t))}_{\bar{h}_i(x,t)} \right] \longrightarrow H$$

s.th. $\frac{dH}{dt} \leq 0$

Basics (Cont'd):

LGA

→ Model ⇝ $\begin{cases} \text{streaming} \\ \text{collision} \end{cases}$ – constraints: mass conservation etc

→ Equilibrium stochastic, maximal equilibrium possible Fermi-Dirac eq.
↳ H-Theorem

→ Short comings.

→ (Intermediate Models)

LBM (Derivation) — should know how

→ LB equation. → should write down.

→ moments $\begin{pmatrix} \sum f_i = \rho \\ \sum \underline{c}_i f_i = \rho \underline{u} \end{pmatrix}$

→ Multiscale expansion → should know concept perturbation, Taylor expansion around the equilibrium

→ Viscosity — the parameter

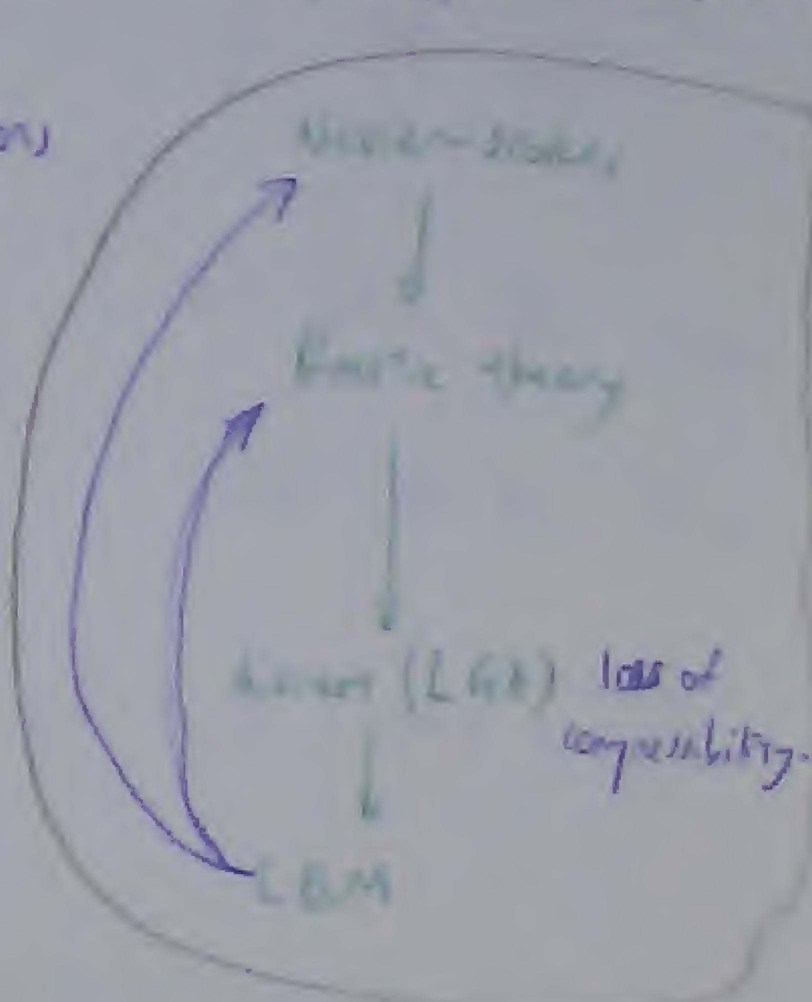
$\Downarrow$

NS ② small compressibility approx. (incomp. NS)

– Stability — how and stability infer

– Boundary conditions

– H-Theorem.



$$f^{(q)} = \arg\min \left\{ H^{(q)}(f) : \rho = \sum f_i^{(0)} ;\ \sum \underline{c}_i f_i^{(0)} \right\} = \rho \underline{u}$$

introduce Lagrangian:

$$H_L := \sum_i h_i(f_i) - a\left(\sum f_i - \rho\right) + \underline{b} \cdot \left(\sum \underline{c}_i f_i - \rho \underline{u}\right)$$

optimality condition:

$$\frac{\partial H_L}{\partial f_i} = h_i'(f_i) - a - \underline{c}_i \underline{b} \stackrel{!}{=} 0$$

$$\Rightarrow f_i^{(0)} = (h_i')^{-1}(a + \underline{b} \cdot \underline{c}_i) \qquad \sum_i f_i^{(0)} = \rho \qquad \sum_i \underline{c}_i f_i^{(0)} = \rho \underline{u}$$

Show: H is non-increasing during collision:

$$f_i(t) + \omega\left(f_i^{(0)}(t) - f_i(t)\right) = f(t+1)$$

Recall: fundamental theorem of calculus:

$$\int_0^1 \frac{\partial}{\partial s} g(t+s)\, ds \underset{t+s=\xi}{=} \int_t^{t+1} g'(\xi)\, d\xi = g(t+1) - g(t)$$

$$\boxed{\text{Define: } f_i(t+s) = f_i(t) + s\omega\left(f_i^{(0)}(t) - f_i(t)\right)} \quad 0 \leq s \leq 1 \qquad \sum f_i(t+s) = \rho(t+s),\ \rho\underline{u} \text{ similar}$$

Let $0 < \omega < 1$ generally $0 < \omega < 2$

Then

$$\bar{h}_i(t+1) - \bar{h}_i(t) = h_i(f_i(t+1)) - h_i(f_i(t)) = \int_0^1 \frac{\partial}{\partial s}\left\{ h_i(f_i(t+s)) \right\} ds$$

$$= \int_0^1 \frac{\partial}{\partial s}\left\{ h_i(f_i(t+s)) \right\} + a\frac{\partial}{\partial s}\underbrace{\left(\sum f_i - \rho\right)\Big|_{t+s}}_{=0} + \underline{b}\frac{\partial}{\partial s}\left(\sum \underline{c}_i f_i - \rho\underline{u}\right)\Big|_{t+s} ds$$

$$= \int_0^1 \left(\frac{\partial h_i}{\partial f_i} - a\frac{\partial}{\partial f_i}\left(\sum f_i - \rho\right) - \underline{b} \cdot \frac{\partial}{\partial f_i}\left(\sum \underline{c}_i f_i - \rho \underline{u}\right) \right) \frac{d}{ds} f(t+s)\, ds$$

$$= \int_0^1 \left(h_i' - a - \underline{b} \cdot \underline{c}_i\right) \omega \left(f_i^{(0)} - f_i\right)\Big|_{t+s} ds$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\tfrac{1}{2} - \tfrac{1}{\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\tfrac{1}{2} - \tfrac{1}{\omega}\right)\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum c_{i,\alpha} c_{i,\beta} c_{i,\gamma} f_i^{(0)}$$

$$P_{\alpha\beta} = \partial_\alpha p = \partial_\beta \rho c_s^2 + O(h^2) \qquad f_i^{(0)} \approx \rho w_i \left(1 + \frac{c_{i,\alpha} u_\alpha}{c_s^2}\right) + O(h^2)$$

$$= \partial_\beta^{(1)}\partial_\gamma^{(1)} \sum \underbrace{c_{i,\alpha} c_{i,\beta} c_{i,\gamma} \rho w_i}_{\text{odd moments vanish}} \left(1 + \frac{c_{i,\sigma} u_\sigma}{c_s^2}\right)$$

$$\left[\text{Now: } \sum w_i c_{i,\alpha} c_{i,\beta} c_{i,\gamma} c_{i,\sigma} = c_s^4 (\delta_{\alpha\beta}\delta_{\gamma\sigma} + \delta_{\alpha\gamma}\delta_{\beta\sigma} + \delta_{\alpha\sigma}\delta_{\beta\gamma})\right]$$

$$= c_s^2 \begin{cases} 3\partial_1^{(1)}\partial_1^{(1)}(\rho u_1) + 2\partial_1^{(1)}\partial_2^{(1)}(\rho u_2) + \partial_2^{(1)}\partial_2^{(1)}(\rho u_1), & \alpha = 1 \\ \partial_1^{(1)}\partial_1^{(1)}\partial(\rho u_2) + 2\partial_1^{(1)}\partial_1^{(1)}(\rho u_1) + 3\partial_1^{(1)}\partial_2^{(1)}(\rho u_2), & \alpha = 2 \end{cases}$$

$$= c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

Note: mass eqn: $\partial_\beta^{(1)} c_s^2 = c_s^2 \partial_t^{(1)} \rho = c_s^2 \partial_\beta^{(1)}(\rho u_\beta + O(\varepsilon))$

~~$\partial_t \partial_\beta (u_\alpha)$~~

$$\partial_t^{(2)}(\rho u_\alpha) - \Delta t\left(\tfrac{1}{2} - \tfrac{1}{\omega}\right) c_s^2 \partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta) + \Delta t\left(\tfrac{1}{2} - \tfrac{1}{\omega}\right) c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\tfrac{1}{2} - \tfrac{1}{\omega}\right) c_s^2 \left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + \partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

$$\varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)} = \partial_t$$

$$\Rightarrow \partial_t \rho + \partial_\beta(\rho u_\beta) = 0$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) + \partial_\alpha p = \Delta t\left(\tfrac{1}{\omega} - \tfrac{1}{2}\right) c_s^2 \underbrace{\left(\partial_\beta\partial_\beta(\rho u_\alpha) + \partial_\alpha\partial_\beta(\rho u_\beta)\right)}_{\to \partial_\beta\partial_\beta(\rho u_\alpha)}$$

$u_\alpha \to 0$

$\rho = \text{const.}$

In vector form, this is $\nabla^2 \underline{u}$

$\frac{1}{\Delta t}$ ... $= \partial_t (\rho u_\alpha) + \partial_\alpha^{(1)} p + \partial_\beta^{(1)}(\rho u_\alpha u_\beta)$

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1

Numerics of LBM

- Setup of LBM simulations
- Boundary conditions
- Stability.

1. Setup of LBM sim.

$0 < \omega < 2$ — tuning viscosity

$$\text{LBM}: \quad f_i(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega\left(f_i^{(eq)}(\underline{r}, t) - f_i(\underline{r}, t)\right); \quad i = 0, \dots, 8$$

two cases:

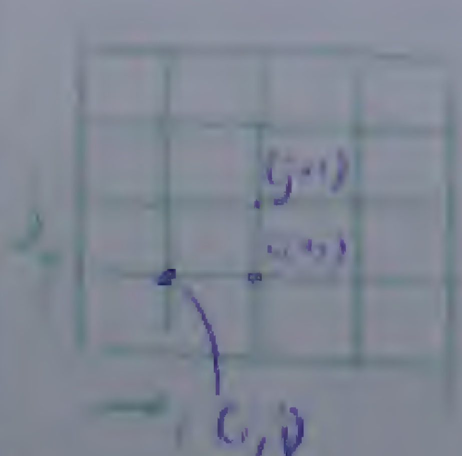
- Time-dependent
- Steady case

} treated the same

until $\|u_{n+1} - u_n\| < \varepsilon$

$$f_i(\underline{r}+\underline{c}_i) = f_i(\underline{r}) + \omega\left(f_i^{(eq)}(\underline{r}) - f_i(\underline{r})\right)$$

Recall: grid topology



save $f_i^{(eq)}, f_i$ as

$f(k, \underbrace{i,j}_{\text{location}})$ $\quad k = 0, \dots, 8$; $\quad i,j = 0, \dots, N$

$\rho(i,j)$ etc

$\underline{u} = (u, v)$, $u(i,j)$, $v(i,j)$

Code outline

$(\rho_0, \underline{u}_0, \omega)$ — initial conditions

$f_i^{(eq)}(\rho_0, u_0) \longrightarrow f_* = f^{(eq)}$

do $n = 0, 1, 2, 3, \dots$

- $(\rho, \underline{u}) = \text{macro var}(f)$ $\quad \rho = \sum f_i$, $\quad u = \frac{1}{\rho}\sum c_i f_i$
- $f^{(eq)} = \text{compute Eq}(\rho, \underline{u})$
- $f \leftarrow \text{collision}(f, f^{(eq)})$ $\quad f \leftarrow f + \omega(f^{(eq)} - f)$ $\quad \leftarrow$ apply source term
- $f \leftarrow \text{apply b.c.}(f)$
- $f \leftarrow \text{streaming}(f)$ $\quad f_i(r + c_i, t+1) = f(r, t)$ $\quad$ collision term already add

$$= \partial^{(1)}(\rho u_\alpha) + \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\alpha} + \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right)\partial^{(1)}\partial_\alpha^{(1)} \ldots$$

Setup of LBM Simulation

given dimensional variable, kinematic viscosity

ρ_{ref}^*, u_{ref}^*, ν^*, L dimensionless length scale

Recall

$$f^{(eq)} \propto e^{\frac{-(u-c)^2}{2\boxed{RT}(c_s^2)}}$$

Pick Reference Mach number

e.g. $M = 0.01 \Rightarrow (c_s^*)^* = \frac{u_{ref}}{M}$

$C_o^* = \sqrt{3}\, C_s^*$ (lattice D2Q9)

Now

$\Delta x^* = \frac{L}{N}$

since $\Delta x^* = C_o^* \Delta t^*$

$\Rightarrow \Delta t^* = \frac{\Delta x^*}{C_o^*}$

$= \quad t = \frac{t^*}{\Delta t^*} \quad (\Rightarrow \Delta t^* = 1)$

Non-dimensionalize:

Eq $\quad c_\alpha = \frac{c_\alpha^*}{C_o^*} \quad u_\alpha = \frac{u_\alpha^*}{C_o^*} \quad c_s^* = \frac{c_s^*}{C_o^*} \quad \rho = \frac{\rho^*}{\rho_{ref}^*} \quad f = \frac{f^*}{\rho_{ref}^*}$ non-dimensionalize everything

$$\Rightarrow \frac{(f^{(eq)})^*}{\rho_{ref}^*} = \frac{\rho^*}{\rho_{ref}^*} w_i \left\{ 1 + \frac{c_i^* u^*}{(c_s^*)^2} + \frac{1}{2}\frac{(c_i^* \cdot u^*)}{(c_s^*)^4} - \frac{1}{2}\frac{(u^*)^2}{(c_s^*)^2} \right\} \quad \frac{(c^*)u^*}{(c_s^*)^2} = \frac{c \cdot u}{c_s^2}$$

$\Rightarrow \rho w_i \{1 \ldots$ drop the $*$ $\}$

if $\nu = \frac{\nu^*}{(C_o^*)^2 \Delta t^*}$ from small, $\nu = \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right) c_s^2$

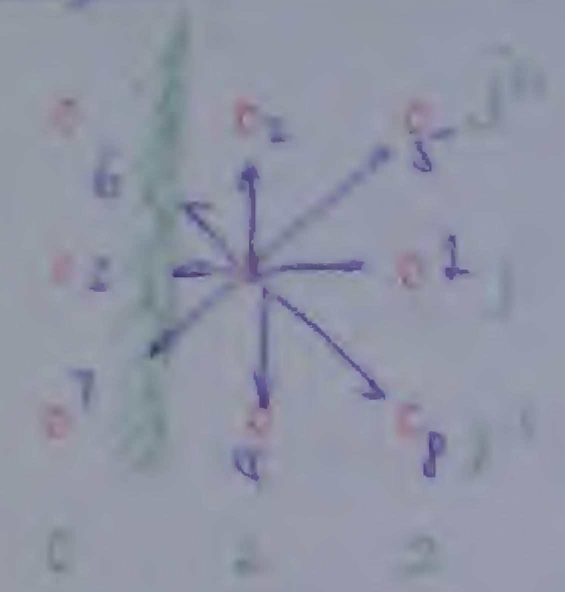
$\Rightarrow \frac{\nu}{\Delta t c_s^2} = \frac{1}{\omega} - \frac{1}{2}$

$$\Rightarrow \boxed{\omega = \frac{1}{\frac{\nu}{\Delta t c_s^2} + \frac{1}{2}}}$$

Now $\frac{\nu}{\Delta t\, c_s^2} = \frac{\nu}{c_s^2} = \frac{\nu^*}{(C_o^*)^2 \Delta t^*}\frac{(C_o^*)^2}{(C_s^*)^2}$

$=1$

Boundary Conditions



assumption,
after collision step

pseudo-'bcs', with ghost cells

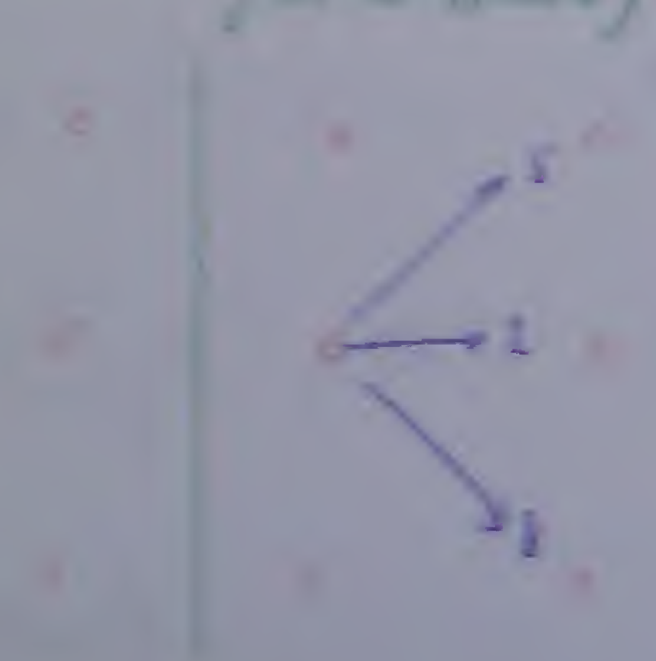
$f_{7,0,j+1} = f_{6,1,j}$

$f_{3,0,j} = f_{2,1,j}$

$f_{5,0,j-1} = f_{7,1,j}$

Flux Boundary Conditions

inflow boundary



Have (u_0, v_0) at inflow

unknowns: ρ, f_1, f_5, f_8

Have: moment relations

$$\left.\begin{aligned} \underline{u} &= \frac{1}{\rho}\sum c_i f_i \\ \rho &= \sum f_i \end{aligned}\right\} \text{three relations}$$

extra equation:

$$f_1 - f_1^{(eq)} = f_3 - f_3^{(eq)}$$

$$\Rightarrow f_1 = f_3 - (f_3^{(eq)} - f_1^{(eq)})$$

$$\Rightarrow f_1 = f_3 + \frac{2}{3}\rho u_0$$

$$\rho = \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{1 - u_0}$$

$$\Rightarrow f_5 = f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho u_0$$

$$\Rightarrow f_8 = f_6 - \frac{1}{2}(f_4 - f_2) + \frac{1}{6}\rho u_0$$

= Stability Analysis

Setup: ⊛ Assume infinite lattice

⊛ $\rho_0, \underline{u}_0$ be uniform at $t=0$

i.e. $\rho(\underline{x},0) = \rho_0$, $\underline{u}(\underline{r},0) =: \underline{u}_0$ $\Big\} \to f_i^{(eq)}(\underline{r},0) =: f_{i,0}^{(eq)} = \text{const.}$

⊛ Assume $f_i(\underline{x},0)$ is uniform @ $t=0$ (e.g. $f_i = f_i^{(eq)}$)

i.e. $f_i(\underline{x},0) = f_{i,0} = \text{const.}$ $\left(\sum f_i = \rho_0 \quad \sum c_i f_i = \rho_0 \underline{u}_0\right)$

$\boxed{\text{Consider LBM @ } t=0}$

$$f(\underline{r}+\underline{c},1) = f_i(\underline{r},0) + \omega\left(f_{i,0}^{(eq)} - f_{i,0}\right) =: f_{i,1} \quad (1)$$

[illegible] no sense where you go, $\underline{r}+\underline{c}$ or $\underline{r}$, the values are the same, hence the $\underline{c}$ in LBM can be dropped

$$\Rightarrow f_{i,1} = (1-\omega) f_{i,0} + \omega f_{i,0}^{(eq)} \quad ⊛$$

$$\Rightarrow \sum f_{i,1} = (1-\omega)\underbrace{\sum f_{i,0}}_{\rho} + \omega \underbrace{\sum f_{i,0}^{(eq)}}_{\rho}$$

[illegible] $\rho_0 u_0$

[illegible] be ρ [illegible]
[illegible] constant.

Subtract $f_{i,0}^{(eq)}$ from (1)

$$\Rightarrow \tilde{f}_{i,1} = f_{i,1} - f_{i,0}^{(eq)} = (1-\omega) f_{i,0} + (\omega - 1) f_{i,0}^{(eq)}$$

$$= (1-\omega)\underbrace{\left(f_{i,0} - f_{i,0}^{(eq)}\right)}_{\tilde{f}_{i,0}}$$

$$\Rightarrow \tilde{f}_{i,1} = (1-\omega)\tilde{f}_{i,0}$$

⊛ $\to f_{i,2} = (1-\omega) f_{i,1} + \omega f_{i,1}^{(eq)}$ [illegible] $\to$ subtract $f_{i,0}^{(eq)} \to \tilde{f}_{i,2} = (1-\omega)\tilde{f}_{i,1} = (1-\omega)^2 \tilde{f}_{i,0}$ Recursion proof

$$\Rightarrow \tilde{f}_{i,k} = (1-\omega)^k \tilde{f}_{i,0}$$

Need $|1-\omega| \leq 1$

$\Rightarrow 0 \leq \omega \leq 2$

LBM

(1) 3rd Feb 2017

(i) linear Stability Analysis.

(ii) H - Theorem

Fourier Analysis (Von Neumann test)

Example.

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad x \in [0, 2\pi),\ a > 0$$

$$u(x,t) = u(x+2\pi, t) \quad \forall t$$

$$u(x,0) = u_0(x)$$

$$u_0(x+2\pi) = u(x)$$

Finite Difference:

$$g_h := \{ih : i = 0, \ldots, N;\ hN = 2\pi\}$$

$$g_\tau := \{n\tau : n = 0, \ldots, M;\ M\tau = T\}$$

$[0, 2\pi) \times [0, T]$

$$u_t(x_i, t^n) = \frac{u_i^{n+1} - u_i^n}{\tau} + O(\tau)$$

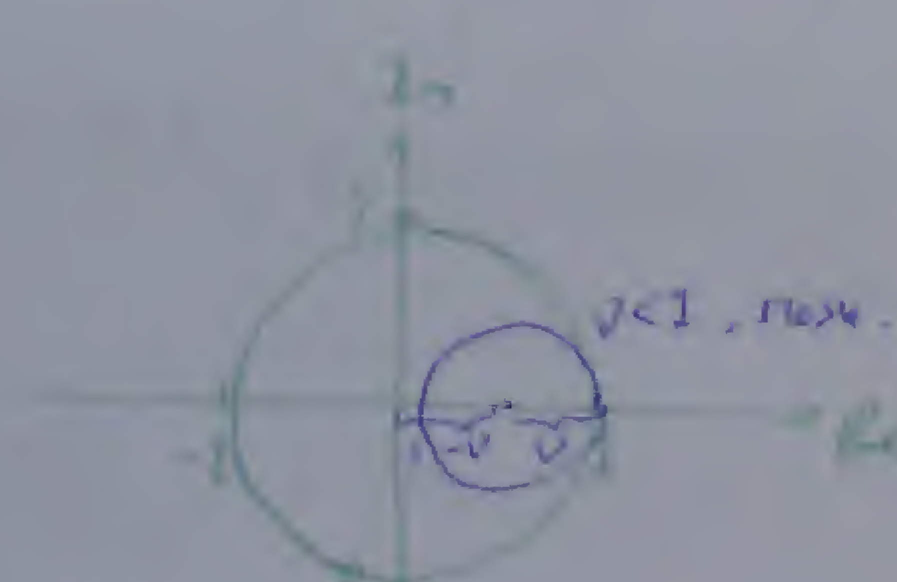
$$u_i^n = u(x_i, t^n)$$

$$u_x = \frac{u_i^n - u_{i-1}^n}{h} + O(h)$$

$$\Rightarrow \frac{u_i^{n+1} - u_i^n}{\tau} + a\frac{u_i^n - u_{i-1}^n}{h} = 0 \qquad \Rightarrow u_i^{n+1} = u_i^n - \nu(u_i^n - u_{i-1}^n);\ \nu = \frac{a\tau}{h}$$

Fourier:

$$u_i^n = \sum_{k=0}^{N-1} c_k^n e^{\imath k i h} \quad *$$



Substitute into scheme:

$$c_k^{n+1} e^{\imath k i h} = c_k^n\left(e^{\imath k i h} - \nu\left(e^{\imath k i h} - e^{\imath k(i-1)h}\right)\right)$$

$$\Rightarrow \left|\frac{c_k^{n+1}}{c_k^n}\right| = \left|1 - \nu(1 - e^{-\imath k h})\right| \leq 1 \quad \text{bounded by 1 means} \quad e^{\imath\theta} = \cos\theta + \imath\sin\theta$$

$$1 - \nu + \nu e^{-\imath k h}$$

unit circle with radius ν

shifted to $1-\nu$ away from zero

Application to LBM

$$f_i(x+c_i, t+1) = \underbrace{f_i(x,t) + \frac{1}{\tau}\left(f_i^{(eq)}(x,t) - f_i(x,t)\right)}_{g}$$

"nonlinear" comes from $f_i^{(eq)}$

$f_i^{(eq)} = f_i^{(eq)}(\rho, \underline{m})$; $\rho = \sum_i f_i$; $\underline{m} = \sum_i c_i f_i$

$f_i^{(eq)} = f_i^{(eq)}(\rho(f), m(f))$; $f = [f_0 \ldots f_8]^T$

Apply von Neumann $\Rightarrow$ linearize!

$f_i = \overline{f_i^{(eq)}} + f_i'$

const + f(x)

$$\overline{f^{(eq)}} + \frac{1}{\tau}\overbrace{\left(f_i^{(eq)}(\rho(\overline{f^{(eq)}}), m(\overline{f^{(eq)}}))_i - \overline{f_i^{(eq)}}\right)}^{=0}$$

$$\overline{f_i^{(eq)}} + f_i'(x+c_i, t+1) = g_i(\overline{f^{(eq)}}) + \left.\frac{\partial g_i}{\partial f_j}\right|_{\overline{f^{(eq)}}} f_j'$$

difference first then substitute with $\overline{f^{(eq)}}$

$$\Rightarrow \overline{f_i^{(eq)}} + f_i'(x+c_i, t+1) = \cancel{\overline{f^{(eq)}}} + f_i' + \frac{1}{\tau}\left(\frac{\partial f_i^{(eq)}}{\partial f_j} f_j' - f_i'\right)$$

$$f_i'(x+c_i, t+1) = G_{ij} f_j'(x,t) \; ; \; G_{ij} = \left(1 - \frac{1}{\tau}\right)\delta_{ij} + \frac{1}{\tau}\frac{\partial f_i^{(eq)}}{\partial f_j}$$

$$f_i^{(eq)} = w_i \rho \left\{1 + 3 c_i \cdot u + \frac{9}{2}(c_i \cdot u)^2 - \frac{3}{2}u^2\right\}$$

$$\left[\rho = \sum f_i \quad \rho \underline{u} \equiv \underline{m} = \sum c_i f_i = c_0 f_0 + c_1 f_1 + \ldots + c_8 f_8\right]$$

$$\Rightarrow f_i^{(eq)} = w_i \left\{\rho + 3 c_i \cdot \underline{m} + \frac{9}{2} \cdot \frac{1}{\rho} c_i \cdot (\rho \underline{u})^2 - \frac{3}{2} \cdot \frac{1}{\rho}(\rho \underline{u})^2\right.$$

$\rho = \sum f_j$

$$\frac{\partial f_i^{(eq)}}{\partial f_j} = w_i \left\{1 + 3 c_i \cdot c_j + \frac{9}{2}\left(-\frac{1}{\rho^2}\right)(c_i \cdot (\rho u))^2 + \frac{9}{2}\frac{1}{\rho} 2 (c_i \cdot (\rho u))(c_i \cdot c_j) + \frac{3}{2}\left(-\frac{1}{\rho^2}\right)|\rho u|^2\right.$$

$$\left. + \frac{3}{2} \cdot \frac{1}{\rho} 2 \rho \underline{u} \cdot c_j \right\}$$

note, in the c_i, it is independent of ρ

$$= w_i \left\{1 + 3 c_i \cdot c_j + \frac{9}{2}\left(2 (c_i \cdot c_j)(c_i \cdot \underline{u}) - (c_i \cdot \underline{u})^2\right) + \frac{3}{2}\left(2 c_j \cdot \underline{u} - |\underline{u}|^2\right)\right.$$

$$f_i'(x,t) = \sum_{k_x, k_y} F(k_x, k_y, t)\, e^{\hat{\imath} \underline{k} \cdot \underline{x}} \; ; \; \underline{k} = [k_x \; k_y]^T$$

Boundaries!

$$e^{\hat{\imath} \underline{k} \cdot (\underline{x} + c_i)} F_i(k_x, k_y, t+1) = G_{ij} F_j(k_x, k_y, t)\, e^{\hat{\imath} \underline{k} \cdot \underline{x}}$$

$$\Rightarrow F_i(k_x, k_y, t+1) = \underbrace{G_{ij}\, e^{-\hat{\imath} \underline{k} \cdot c_i}}_{\Gamma_{ij}} F_j(k_x, k_y, t)$$

Read stability analysis on LBM (prepared by Prof. Mayo)

$$f_i(t+s) - f^{(0)}(t) = f_i(t) - f_i^{(0)}(t) + s\omega\left(f_i^{(0)}(t) - f_i(t)\right) = (-1+s\omega)\left(f_i^{(0)}(t) - f_i(t)\right)$$

$$\Rightarrow f_i^{(0)} - f_i = \frac{f_i(t+s) - f_i^{(0)}(t)}{s\omega - 1} = \frac{f_i^{(0)}(t) - f_i(t+s)}{1 - s\omega}$$

$$(*) = \tilde{h}(t+1) - \tilde{h}(t)$$

$$= \underbrace{\int_0^1 \underbrace{\left(h_i'(f(t+s)) - h_i'(f^{(0)}(t))\right)}_{\Delta h_i'} \underbrace{\frac{\omega}{1-s\omega}}_{\geq 0} \underbrace{\left(f_i^{(0)}(t) - f_i(t+s)\right)}_{-\Delta f} ds}_{\leq 0}$$

h_i convex

$$\Rightarrow \frac{\Delta h_i'}{\Delta f} \geq 0 \quad \Big| \cdot \underbrace{(\Delta f)^2}_{\geq 0}$$

$$\Leftrightarrow \Delta f \cdot \Delta h_i' \geq 0$$

$$\Leftrightarrow -\Delta f \, \Delta h_i' \leq 0$$

$$(h_i')^{-1}(x) = a + bx + cx^2 = f_i^{(0)} \quad ; \quad x = \underbrace{a}_{a = a(\rho, u)} + \underbrace{\underline{b}}_{b(\rho, u)} \cdot \underline{c}_i \qquad \sum f_i^{(0)} = \rho \qquad \sum f_i^{(0)} = \rho \underline{u}$$

[illegible]

Exam:

→ Continuum mechanics:

→ Conservation Laws
- conservation laws
- equations of states

[illegible]

→ Kinetic theory
- collision models [illegible]
- Maxwell – Boltzmann
  - H – theorem
- Boltzmann Eq. [illegible]
- Conservation Laws } connected by moments [illegible]
- local thermodynamic equilibrium
  - Euler equations

for equilibrium [illegible]

- BGK eq. [illegible]
- Chapman enskog [illegible] } leads to NS*
  - are there difference with NS.

LBM

② 3rd Feb 2017

Recall: Boltzmann eq.: $\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = J(f, f)$

H-function $\quad H := \int f \ln f \, d\underline{c}$

H-theorem

$$\frac{dH}{dt} \le 0$$

maxwell-boltzmann dist

$$\frac{dH}{dt} = 0 \iff f \equiv f^{(MB)}$$

$$f^{(MB)} = \operatorname{argmin} \{ H(f) : n = \int_{\mathbb{R}^3} f \, d\underline{c}$$

(ρ, u, T)

$$n\underline{u} = \int_{\mathbb{R}^3} \underline{c} f \, d\underline{c}$$

number density

$$\frac{3}{2} n k_B T = \int_{\mathbb{R}} (\underline{c} - \underline{u})^2 f \, d\underline{c} \}$$

LBM.

$$f_i(\underline{r} + \underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega \left(f_i^{(eq)}(\underline{r}, t) - f_i(\underline{r}, t) \right)$$

$\omega = \frac{1}{\tau}$

$$H = \sum_{i=0}^{N_L} h_i(f_i(\underline{r}, t)) = \sum \tilde{h}_i(\underline{r}, t) \quad ; \tilde{h}_i = h_i \cdot f_i$$

convex function

Look for

$$f_i^{(eq)} = \operatorname{argmin} \{ H(f) : \rho = \sum f_i \, ; \rho u = \sum c_i f_i \}$$

want this to be monotone. (i.e. not grow during collision process!) so that $H(f_i^{(eq)}, f_i)$ will monotonically decrease ~~H(f)~~ $H(f)$

to solve this "look for $f_i^{(eq)}$", we use lagrangian multipliers

Only need to look for collision part, as streaming part just [illegible]